UCRL- 98402
PREPRINT

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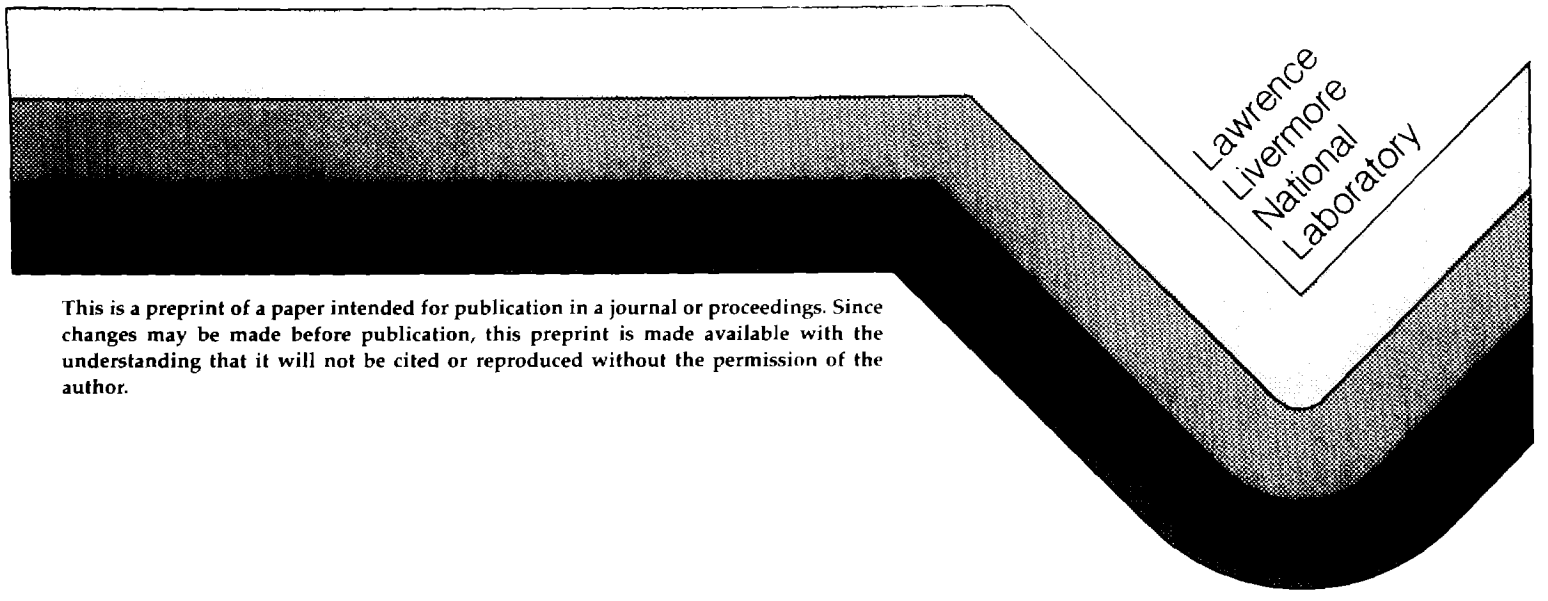
This paper was prepared for submittal to
Western States Section/The Combustion Institute
1988 Spring Meeting
21-22 March 1988
Salt Lake City, Utah

10 March 1988



THE OXIDATION OF N-BUTANE AT LOW AND INTERMEDIATE TEMPERATURES: AN EXPERIMENTAL AND MODELING STUDY

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ABSTRACT

An experimental and modeling study of n-butane oxidation in a static reactor was conducted at temperatures encompassing the negative temperature coefficient region and portions of the low and intermediate temperature regimes. The numerical model employed a detailed chemical kinetic mechanism for n-butane oxidation. Conditions considered in the combined study were temperatures in the range of 554-737 K, an initial pressure of 550 torr, and a molar mixture ratio of 1:20:20.33 n-butane:O_2:N_2. The induction period and stable species concentrations were measured and compared to modeling predictions. The variation in induction period over the region of negative temperature coefficient is well-predicted by the model. The model is also used to analyze the static reactor data of Baker et al. [19,20] who investigated n-butane/H_2/O_2/N_2 mixtures. The agreement between their detailed species concentration measurements and the modeling predictions is good. Modeling calculations identified some of the key reactions at the conditions investigated. Internal H-atom abstractions of the butyl peroxy radicals and subsequent reactions contributed significantly to the major intermediate species that were observed and to the production of reactive OH radicals. Additionally, radical-radical reactions involving the HO_2 radical consumed a significant amount of butyl peroxy radicals and accelerated the overall rate of oxidation.

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INTRODUCTION

Autoignition is an important process that can lead to engine knock in an internal combustion engine [1]. Numerical models with detailed chemical kinetics have been applied to the problem of autoignition and knock [2-10].

We have developed chemical kinetic models to examine experimental results at temperatures above approximately 900 K [11-13]. However, further validation for temperatures below 900 K is required in order to treat properly the chemistry of the end gas. Many studies have established the importance of this lower temperature regime in producing autoignition and knock, including several recent reviews [14,15]. We have included this low temperature range in recent detailed chemical kinetic mechanisms for acetaldehyde and propene [16,17], and the present study extends that model to include n-butane.

Chemistry below 900 K can be divided into two regimes of interest in an engine environment: a low temperature regime dominated by reactions involving alkylperoxy radicals which lead to the production of alkyl hydroperoxides; and an intermediate temperature regime dominated by hydroperoxyl radicals which lead to hydrogen peroxide. These two regimes are usually separated by a region of negative temperature coefficient (NTC) in which the overall reaction rate decreases with increasing temperature. These characteristic reaction regimes are also pressure dependent in that increasing the pressure shifts both regimes and the NTC region to higher temperatures. A detailed kinetic understanding of each of these regimes and the transition from one regime to another is necessary to understand and simulate autoignition and knock.

The present work examines the low to intermediate temperature chemistry for n-butane/air mixtures. N-butane is the first alkane which

exhibits all the essential features of low temperature chemistry which are found in higher alkanes, including isomerizations of alkyl peroxy radicals, a key route which yields significant radical production for most alkanes greater than C_3.

The low temperature chemistry of n-butane has been extensively investigated [18-28] and detailed kinetic mechanisms for its oxidation have been developed recently [11,29,30] These models have been validated for temperatures above approximately 900 K by comparison with data from flow reactors, well-stirred reactors, and flames. This study extends the region of their applicability to low and intermediate temperatures, and computed results are compared to our experimental results in a static reactor and with experimental results of Baker et al. [20,21].

The current study investigates an important regime of n-butane oxidation that has not been examined extensively. In some previous studies, the n-butane has been highly diluted by nitrogen [11], or by hydrogen/oxygen mixtures [20,21]. On the other extreme, other studies considered n-butane/O_2 mixtures with no dilution [23]. Here we investigate a regime in which the reactant concentrations are close to those found in the fuel/air mixture in the end gas of an engine.

EXPERIMENTAL FACILITY

The experimental study of n-butane oxidation was carried out using a conventional low pressure static reactor system, details of which have been described previously [31,32], and only the main features are presented here. The system consists of a cylindrical pyrex reaction vessel (volume 1395 cm^3, diameter 10 cm, surface/volume ratio 0.5 cm^{-1}) located inside a temperature controlled compartment. The pressure inside the vessel is monitored by a Setra Model 204 pressure transducer.

The temperature at the center of the vessel is measured by a Pt/Pt-13% Rh thermocouple constructed of 0.05 mm diameter wire and coated with a thin layer of silica.

The reactants are first premixed in a separate vessel and then rapidly admitted into the preheated, evacuated reaction vessel. At a selected time during the course of the reaction, a sample is withdrawn and injected by way of a gas sampling valve into a Varian 3700 gas chromatograph (GC) for species analysis. The sample is separated on a 2.44 m x 3 mm, 80/100 mesh Porapak Q column using helium carrier gas (20 cc/min). Temperature programming (4 min @ 36 C; 10 C/min to 180 C; 20 min at 180 C) is used to obtain adequate separation of the stable hydrocarbons and oxygenates.

For this work, oxygen (99.6 % pure), nitrogen (99.999 % pure), and n-butane (99.5 % pure) were used as the reactants. Experiments were carried out for a mixture of $n\text{-}C_4H_{10}/O_2/N_2$: 1/2/20.333 molar ratio, at an initial pressure of 550 torr. The initial temperature ranged from 554-737 K, encompassing the NTC region and portions of the low and intermediate temperature regimes.

NUMERICAL MODEL AND REACTION MECHANISM

Reactions in the static reactor have been simulated with the assumptions of constant volume combustion and spatial uniformity over the vessel volume. Overall heat loss to the vessel wall is given by

$$Q = hA(T-T_{wall})$$

where Q is the total heat loss in watts, h is the heat transfer coefficient, A is the inner surface area of the vessel (700 cm^3), and T_{wall} the wall temperature. The value of h (7.0 $Wm^{-2}K^{-1}$) was chosen such that the calculated maximum temperatures most closely matched the

experimental values and is within the range of order of magnitude of heat transfer coefficients for free convection in air (6-30 $Wm^{-2}K^{-1}$) [53].

The chemical kinetic rate equations were integrated in time using the HCT program [33]. The detailed chemical kinetic mechanism employed is based on a high temperature mechanism of n-butane oxidation [3,11] and low temperature mechanisms for propene and acetaldehyde [16,17]. Additional species and reactions have been added to this mechanism to address the oxidation of n-butane at low and intermediate temperatures, as discussed below. The final reaction mechanism is given in the Appendix, showing both forward and reverse rate parameters. Literature values for the rate constants and thermochemistry [34-36] were used whenever possible. When values were unavailable, estimates were made by analogy to similar reactions.

Key Reactions Added to Reaction Mechanism

The most important reactions added to the previous mechanism treated the formation and consumption of butyl peroxy radicals and their subsequent products. The concentration of butyl peroxy radicals is controlled by the equilibrium of the reactions

$$pC_4H_9 + O_2 = pC_4H_9O_2 \quad (1)$$

$$sC_4H_9 + O_2 = sC_4H_9O_2 \quad (2)$$

Equilibrium constants used for these reactions were derived from the results of Slagle et al.[37,38]. They measured the $R+O_2=RO_2$ equilibrium constants at a series of temperatures for C_2H_5, where O_2 adds to a primary site, and for iC_3H_7, where the O_2 adds to a secondary site. Since O_2 adds to both primary and secondary sites on the butyl radical, we have employed their equilibrium constants for $C_4H_9+O_2=C_4H_9O_2$ reactions by analogy. Our fits to the data of

Slagle et al. are: $K_p(1) = 1.64 \times 10^{-8} \exp(35.2 \text{ kcal/RT})$ and $K_p(2) = 2.78 \times 10^{-9} \exp(37.0 \text{ kcal/RT}) \text{ atm}^{-1}$.

One important route for the consumption of butyl peroxy radicals involves internal H-atom abstractions [39-41], which produce peroxides which decompose and yield significant amounts of reactive OH radicals. They occur when the peroxy radical forms a ring-like transition state and result in the internal abstraction of an H-atom to another part of the same molecule. The following is an example of a 1,5p H-atom transfer for the s-butyl peroxy radical:

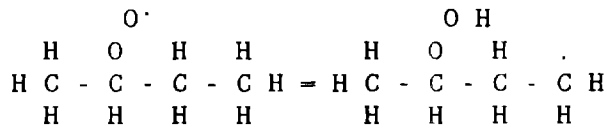


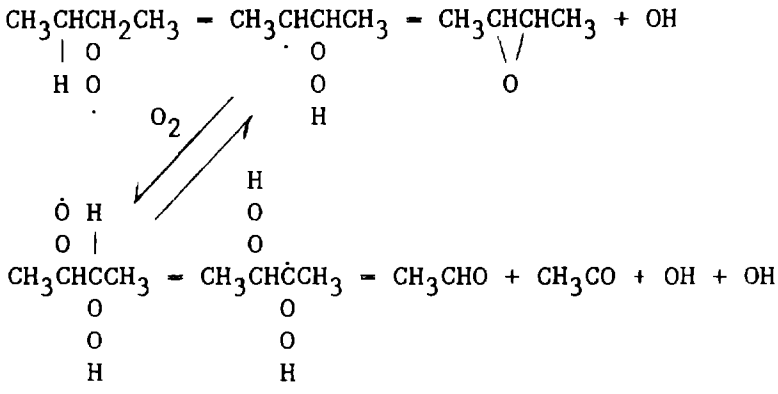
Table I gives all the internal H-atom abstraction reactions considered for n-butane and their rates. We have employed rate constants estimated by Baker et al. [20] and Baldwin and Walker [39]. In order to extract rate constants from their experimental data, the value of the $R+O_2=RO_2$ equilibrium constant was required. We have recalculated the rate constants based on the new values of the equilibrium constants $K_p(1)$ and $K_p(2)$. The current estimates of the rate constants for internal H-atom abstraction given in Table I are approximately an order of magnitude slower than those given by Walker [39]. The reverse rates were calculated from the forward rates and equilibrium constants for the internal H-atom abstraction reactions estimated by Pollard [40].

Another important issue in the oxidation of n-butane and other alkanes is the fate of the QOOH species formed by internal H-atom abstractions:

$$RO_2 = QOOH$$

This species can either decompose, forming an O-heterocycle, or undergo further addition with O_2. The former route leads to the production of one reactive OH radical, and the latter to the eventual production of three

radicals including two OH radicals. The following example shows these two reaction paths for the case of the s-butyl peroxy radical:



The reaction routes shown are analogous to those suggested by Benson [42] for higher alkanes. In the above description, we have extended his suggested path to include the fate of the HOOQ'OOH radical, which is important since it yields two radicals including an OH radical. We have included paths similar to that above for all the QOOH species formed from butyl peroxy radicals.

Other reactions important in consuming butyl peroxy radicals were added to the mechanism. These reactions are of the type:

$$C_4H_9O_2 + HO_2 = C_4H_9O_2H + O_2$$

$$C_4H_9O_2 + HO_2 = C_4H_9O + OH + O_2$$

Although these radical-radical reactions are not important when the fuel is highly diluted, these paths participate significantly under the undiluted conditions found in our static reactor. Baldwin and Walker [38,43] found these types of reactions to be essential in interpreting the results of Euker and Leinroth [27] on n-butane oxidation at about 600 K. We would also expect these reactions to have an important role at undiluted conditions found in the end gas of an engine. In fact, the chemical kinetic model predicted that reaction of butyl peroxy radicals with HO_2 is the most important OH production path for our lowest temperature cases in the static reactor.

We estimated the reaction rate constants of the $C_4H_9O_2$+HO_2 reactions to be 1.0 x 10^{12} $cm^3mole^{-1}s^{-1}$ with no temperature dependence, consistent with the estimates of Benson [42,44] and Walker [39]. This rate constant is 2 times faster than the recommendation of Tsang and Hampson [45] for CH_3O_2+HO_2 which is 4.6 x 10^{10}exp(2.6kcal/RT) $cm^3mole^{-1}s^{-1}$ with an estimated uncertainty of a factor of 5.

Reactions of the type,

$$RO_2 + R'O_2 = RO + R'O + O_2$$

$$CH_3O_2 + CH_3O_2 = CH_3OH + CH_2O + O_2$$

(R, R'= C_4H_9, C_3H_7, C_2H_5, CH_3, CH_3CO) between peroxy radicals consumed a large fraction of these radicals at the low temperature (553 K) condition in our static reactor. The exception was the butyl peroxy radical which was consumed primarily through internal H-atom abstractions. We estimated the rates of the RO_2+RO_2 reactions to be 1.0 x 10^{12} $cm^3mole^{-1}s^{-1}$.

The resonantly stabilized butenyl radical, C_4H_7, was assumed to react with HO_2 with a relatively rapid rate constant of 1.0 x 10^{13} $cm^3mole^{-1}s^{-1}$ via

$$C_4H_7 + HO_2 = C_4H_7O + OH$$

We did not distinguish between the two resonantly stabilized butenyl radicals, $CH_3CHCHCH$ and $CH_2CHCHCH_3$ or the four different types of butenyloxy (C_4H_7O) radicals. The above reaction was the main consumption path for butenyl radicals under all conditions studied here. This reaction is analogous to reaction of HO_2 with other stable radicals such as CH_3 and C_3H_5. There is substantial evidence that this reaction path can be important for resonantly stabilized radicals [16,44,50]. The stable radicals C_3H_5 and CH_3 do not react with O_2 to give HO_2 (eg. C_3H_5+O_2=C_3H_4+HO_2), whereas analogous reaction paths are

major consumers of alkyl radicals at the current conditions [12,46,47,51]. Similarly, we assumed that the radical C_4H_7 does not react with O_2 to produce butadiene. Since C_4H_7, C_3H_5, and CH_3 radicals do not react with O_2 in our numerical model, their concentrations are substantially higher than the alkyl radicals present in the reactive system, allowing the radical-radical reaction with HO_2 to contribute significantly.

One interesting feature of hydrocarbon oxidation in our static reactor is the substantial concentrations of H_2O_2 that are predicted (as high as 1-2 percent), leading to the possibility of alternative paths to thermal decomposition for consumption of H_2O_2. We examined the reaction paths,

$$H_2O_2 + R = HO_2 + RH$$

$$H_2O_2 + RO_2 = HO_2 + RO_2H$$

where the radical R is as previously defined. Using estimated rate data of Tsang and Hampson [45] ($2 \times 10^{14}\exp(0.6\ \text{kcal/RT})$) when R is CH_3, the latter reaction path was found to be the primary consumption path for H_2O_2 for the low temperature (553 K) case in our static reactor, where the rate of thermal decomposition of H_2O_2 is negligible. Inclusion of the $H_2O_2 + RO_2$ reactions reduced the large H_2O_2 concentrations and produced RO_2H which thermally decomposes at a modest rate at 563 K. Thus, we were able to reproduce the relatively fast oxidation rate at this temperature.

Addition reactions between alkenes and OH are a subject of current research. Tully [48] examined alkene/OH/N_2 mixtures in the absence of O_2. He showed that ethene, propene, and 2-butene do not add with OH and produce aldehydic products to any significant extent at temperatures up to approximately 700 K. Consequently, we have not assumed any direct reaction between the butenes and OH in our chemical kinetic mechanism. However when

O_2 is present in the reactive system, the possibility exists for the addition of O_2 to the C_4H_8OH adduct, leading to production of acetaldehyde from 2-butene and propionaldehyde and formaldehyde from 1-butene. These reaction paths, originally proposed by Waddington, are supported by considerable indirect evidence from experimental and modeling studies [16,20,49] and are responsible for a significant amount of the acetaldehyde production and nearly all of the propionaldehyde production in our higher temperature (715 K) case.

RESULTS

Region of Negative Temperature Coefficient

The region of negative temperature coefficient (NTC) is due mainly to a shift in the equilibrium of reactions involving the addition of molecular oxygen to hydrocarbon radicals, R [52]:

$$R + O_2 + (M) = RO_2 \ (+M)$$

In n-butane oxidation, the most important hydrocarbon radicals that participate in these reactions are pC_4H_9, sC_4H_9, nC_3H_7, C_2H_5, and CH_3. At lower temperatures, these RO_2 radicals can undergo internal H-atom abstraction, abstract an H-atom from the fuel, or undergo radical-radical reactions. However, as the temperature is increased, the equilibrium of the $R+O_2=RO_2$ reaction shifts to the left and the concentration of RO_2 decreases. If the RO_2 concentration is sufficiently reduced, the influence of the accelerating paths associated with the RO_2 radical is diminished and the region of NTC is reached (at about 600-640 K in our static reactor for n-butane). In the NTC region, the reaction of alkyl radicals with O_2 gives the alternative products

$$R + O_2 = \text{alkene} + HO_2$$

to a greater extent. These products of $R+O_2$ are not as reactive as the

products obtained at lower temperatures, and the overall rate of reaction slows in the NTC region.

The behavior of the n-butane system over the NTC region is displayed in Fig. 1. The variation in induction period with initial temperature is given by the solid curve and the filled circles. The induction period is defined graphically on a pressure-time plot by obtaining the intersection between the line $P=P_{initial}$ and a tangent to the point of maximum pressure rise. The measured variation in induction period with temperature shown in Fig. 1 is similar to that observed by Dechaux et al. [23] for n-butane/O_2 mixtures. The calculated results are shown as points interconnected with solid lines. The model reproduces the steep variations in measured induction period with temperature quite well. Also, the predicted temperatures that mark the beginning and end of the NTC region closely match the measured temperatures

The variation of the maximum rate of pressure rise, $(dP/dt)_{max}$, with temperature is also given in Fig. 1 (dashed curve and squares). The rate of pressure rise is an interesting quantity since it gives an approximate indication of the overall rate of oxidation. The region of NTC is usually described by the effect of temperature on the overall oxidation rate. The model predicts well the behavior of $(dP/dt)_{max}$ at low temperatures and the temperature at which the NTC region begins. For initial temperatures greater than 680 K, the calculated $(dP/dt)_{max}$ points were not plotted since the reactive mixture undergoes a hot ignition that is not observed experimentally until the initial temperature is increased to a value in excess of about 740 K. The occurrence of these ignitions is very sensitive in the model to the rate at which heat is transferred from the reactive gas to the reactor walls, indicating that the simple Newtonian heat loss model used here, with a constant heat transfer coefficient, may not be

appropriate over the entire range of conditions being studied. The onset of these hot ignitions can be suppressed in the model at temperatures between 680-740 K, where ignitions are not observed experimentally, by increasing the rate of heat transfer in order to examine the reaction progress in this temperature range; but a more complete heat transfer sub-model would improve the entire simulation.

The appearance of pressure spikes superimposed on the pressure histories near the region of NTC in static reactors has been thoroughly documented [41]. They are often referred to as "cool flames". We also observed these pressure spikes experimentally and predicted their occurrence numerically. At the conditions of our investigation, pressure spikes were experimentally observed at temperatures ranging from 563 K to 633 K. The number of pressure spikes increased from one at 563 K to a maximum of three at 596 K and then decreased back to one at 633 K. The modeling results exhibited nearly the same behavior, with the number of pressure spikes being one at 563 K, increasing to a maximum of three at 600 K (see Fig. 2), and decreasing to one at 640 K.

Comparison of Predicted Species Profiles with Experimental Results

In this section, the measured and predicted species concentrations are presented and compared. Figure 3 gives the results for the low temperature case in our static reactor, showing experimental results at 563 K. These are compared with modeling results at the slightly higher temperature of 570 K, the case which best matched the observed overall rate of fuel oxidation. The maxima of calculated and measured species concentrations of CH_3OH, CH_3CHO, and CH_4 agree to within 30 percent. The maximum concentrations of CO_2 and C_2H_4 agree to within a factor of 3. The species histories of 1,2epoxybutane+butyraldehyde+2butanone indicate the

observation and prediction of C_4 O-heterocyclic compounds that result from isomerization of the butyl peroxy radical. These species are plotted as a sum since the GC column was unable to separate them. Other minor species not shown in Fig. 3 (CH_3COCH_3, C_2H_5CHO, C_2H_3CHO, C_3H_6, C_2H_6, 2,3epoxybutane) were measured and predicted in mole fractions less than 0.2 percent.

Next, we discuss the results at an initial temperature of 715 K. The heat transfer rate in the simplified heat transfer sub-model was increased as described previously to suppress the hot ignition and allow a comparison of measured and calculated results as shown in Fig. 4. The computed maximum concentrations of CO, C_2H_4, CH_4, C_4H_8, CH_3CHO, and tetrahydrofuran

agreed with the measured concentrations to within 30 percent. The maximum concentrations of CH_2O, CO_2, and C_3H_6 agreed to within a factor of 3. The reaction path that produced the greatest amount of CH_3CHO was the previously discussed Waddington mechanism of 2-butene. The predicted overall rate of fuel oxidation was faster than the experimental rate, causing the predicted fuel profile to drop more steeply and the intermediate species profiles to be shaped more narrowly than the experimental profiles.

The experimental and modeling results showed a significant shift in product distribution when the initial temperature is raised from low to intermediate temperatures. There is a general shift from oxygenated product species at low temperatures to alkenes and methane at intermediate temperatures. When the initial temperature is raised from 563 K to 715 K, the concentrations of acetaldehyde, formaldehyde, and methanol decrease significantly and the concentrations of butene, propene, ethene, and methane increase substantially. This shift in product distribution can be

traced to the shift in the equilibrium of the $R+O_2=RO_2$ reactions, which reduces the contribution of RO_2 radicals and their subsequent reactions.

We applied our chemical kinetic model to the static reactor environment studied by Baker et al. [19,20]. They examined the oxidation of small amounts of n-butane added to H_2/O_2 mixtures at 753 K, obtaining a thorough description of the temporal histories of nearly all the intermediate products. The calculated species profiles are compared to their measured profiles in Fig. 5. The species profiles are plotted with respect to the amount of n-butane consumed, which is the same format in which the experimental data were reported. The measured and calculated maximum concentrations of each species agree to within 30 percent. The agreement for the 1,2-epoxybutane and the 2-butene is very good. The predicted concentrations of the alkenes, C_3H_6 and C_2H_4 are low compared to the measured values. The concentrations of these species are sensitive to any transient temperature rise in the static reactor since they are formed from the highly endothermic decomposition of the butyl radicals. We believe that there may be a temperature rise above the initial temperature in the static reactor during the experiment, which would explain the relatively high measured concentrations of these alkenes. Tetrahydrofuran was produced in significant quantities both in the experiment and in the numerical model. Its production demonstrates the importance of internal H-atom abstractions of the butyl peroxy radical, which is the only path forming tetrahydrofuran.

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory Contract No. W-7405-ENG-48 and the U.S. Army Research Office Contract No. DAAG 29-85-K-0253.

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Table I

Internal H-atom abstractions

Reaction rates in cm^3-mole-sec-kcal units, $k=AT^n exp(-E_a/RT)$

	Reaction	Forward rate log A	n	E_a	Reverse rate log A	n	E_a
1.	$pC_4H_9O_2 = CH_2CH_2CH_2CH_2O_2H$	8.34	0.0	19.00	7.86	0.00	11.00
2.	$pC_4H_9O_2 = CH_3CHCH_2CH_2O_2H$	8.72	0.0	17.30	7.93	0.00	12.90
3.	$pC_4H_9O_2 = CH_3CH_2CHCH_2O_2H$	8.81	0.0	20.40	8.51	0.00	15.90
4.	$sC_4H_9O_2 = CH_2CH_2CHO_2HCH_3$	8.72	0.0	20.90	8.23	0.00	12.90
5.	$sC_4H_9O_2 = CH_3CHCHO_2HCH_3$	8.81	0.0	20.40	8.51	0.00	15.90

FIGURE CAPTIONS

Fig. 1. The variation of maximum rate of pressure rise, $(dP/dt)_{max}$, (--, □) and induction period (—, ●) with initial reactor temperature for n-butane oxidation. The curves represent the computed results using the numerical model, and the symbols represent the experimental results.

Fig. 2. Pressure history predicted by chemical kinetic model at an initial temperature of 600 K.

Fig. 3. Concentrations of intermediate species for an initial temperature of 563 K. Curves indicate computed results using the detailed mechanism, and symbols represent our experimental results. (Top: — ●, C_4H_{10}; — ○, CO; -- □, CO_2; · — △, CH_2O; - — ◇, CH_3OH x3. Bottom: - — ◇, C_4H_8 x2; — ●, CH_3CHO; · — ○, CH_4; -- □, C_2H_4 x2; — , 1,2epoxybutane+butyraldehyde+2butanone).

Fig. 4. Concentrations of intermediate species for an initial temperature of 715 K. Curves indicate computed results using the detailed mechanism, and symbols represent our experimental results. (Top: — ●, C_4H_{10}; — ○ CO x0.5; --,□CO_2; · — ■, C_2H_4 x2; · — △, CH_4. Bottom: - — ■, C_4H_8; · — □, C_3H_6; — ●, CH_3CHO; -- △, CH_2O; -- ○, tetrahydrofuran x30.)

Fig. 5. Concentrations of intermediate species for an initial temperature of 753 K. Curves indicate computed results using the detailed mechanism, and symbols represent experimental results of Baker et al. [19]. The initial conditions are H_2=140 torr, O_2=355 torr, and nC_4H_{10}=5 torr. (Top: — ▽, CH_3CHO x0.5; -- △, 1,2epoxybutane; - — ○, 2,3epoxybutane; — □, tetrahydrofuran x3; · — ◇ 2methyloxetan. Bottom: - — ■, $1C_4H_8$; — ○, $2C_4H_8$; — ●, C_3H_6; · — □, C_2H_4 x1/3; -- △, CH_2O x0.1).

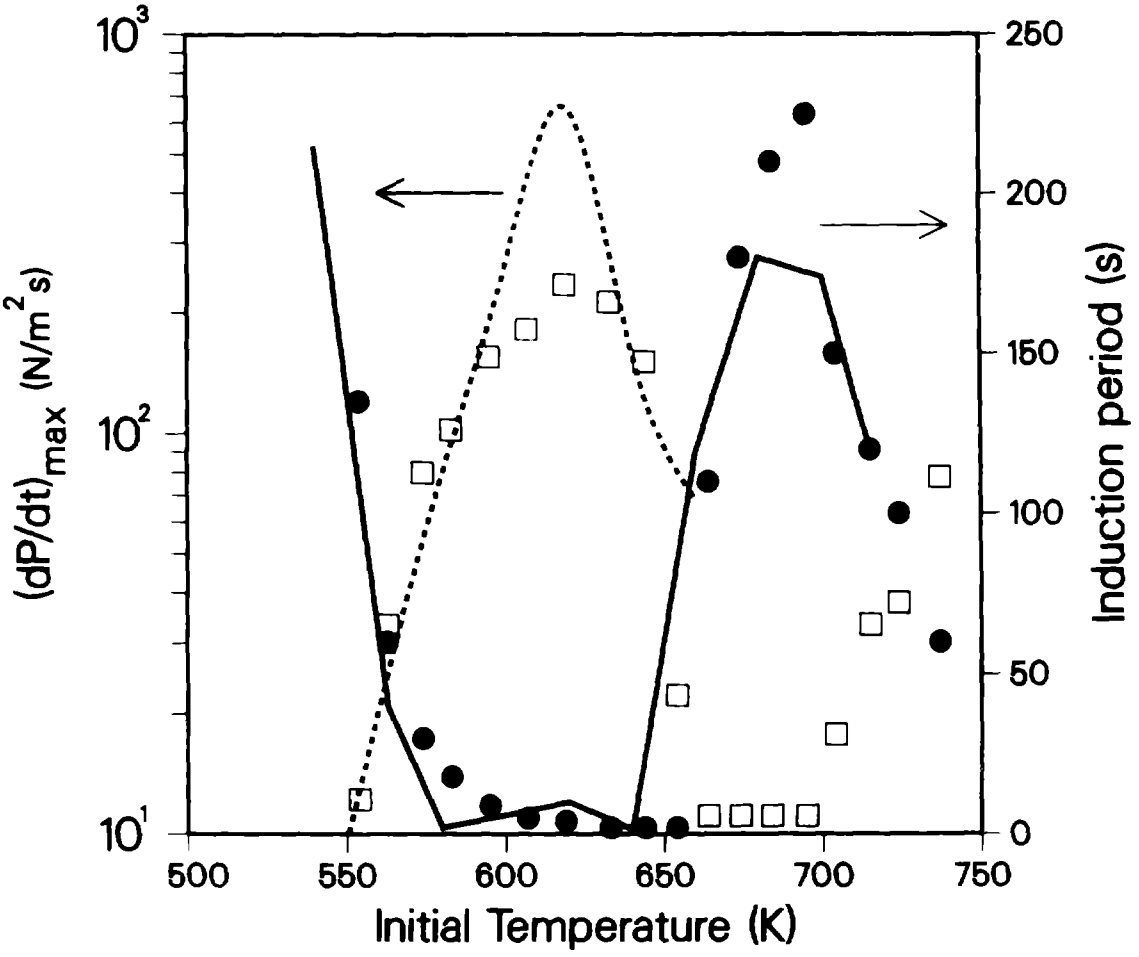
10^3
10^2
10^1
$(dP/dt)_{max}$ (N/m^{2}s)
250
200
150
100
50
0
Induction period (s)
500
550
600
650
700
750
Initial Temperature (K)

Fig. 1

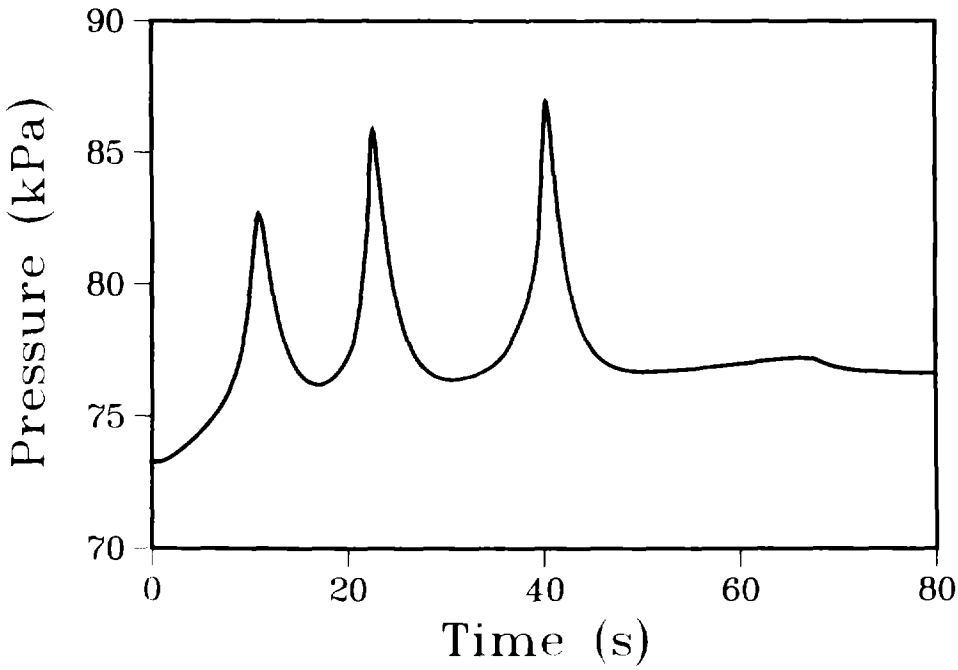

Fig. 2

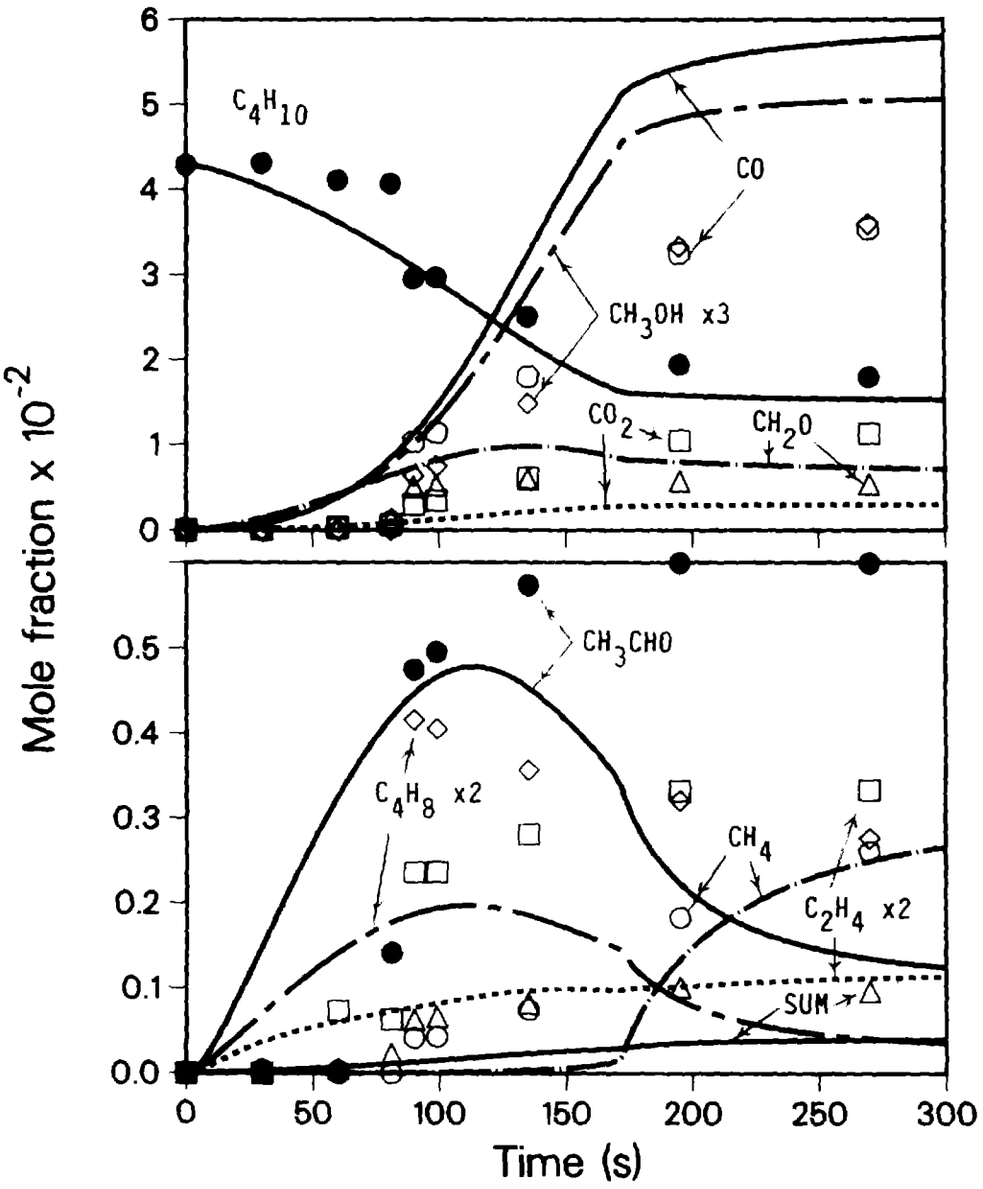
Mole fraction x 10^{-2}
C_4H_{10}
CO
CH_3OH x3
CO_2
CH_2O
CH_3CHO
C_4H_8 x2
CH_4
C_2H_4 x2
SUM
Time (s)
0
50
100
150
200
250
300
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3
4
5
6

Fig. 3

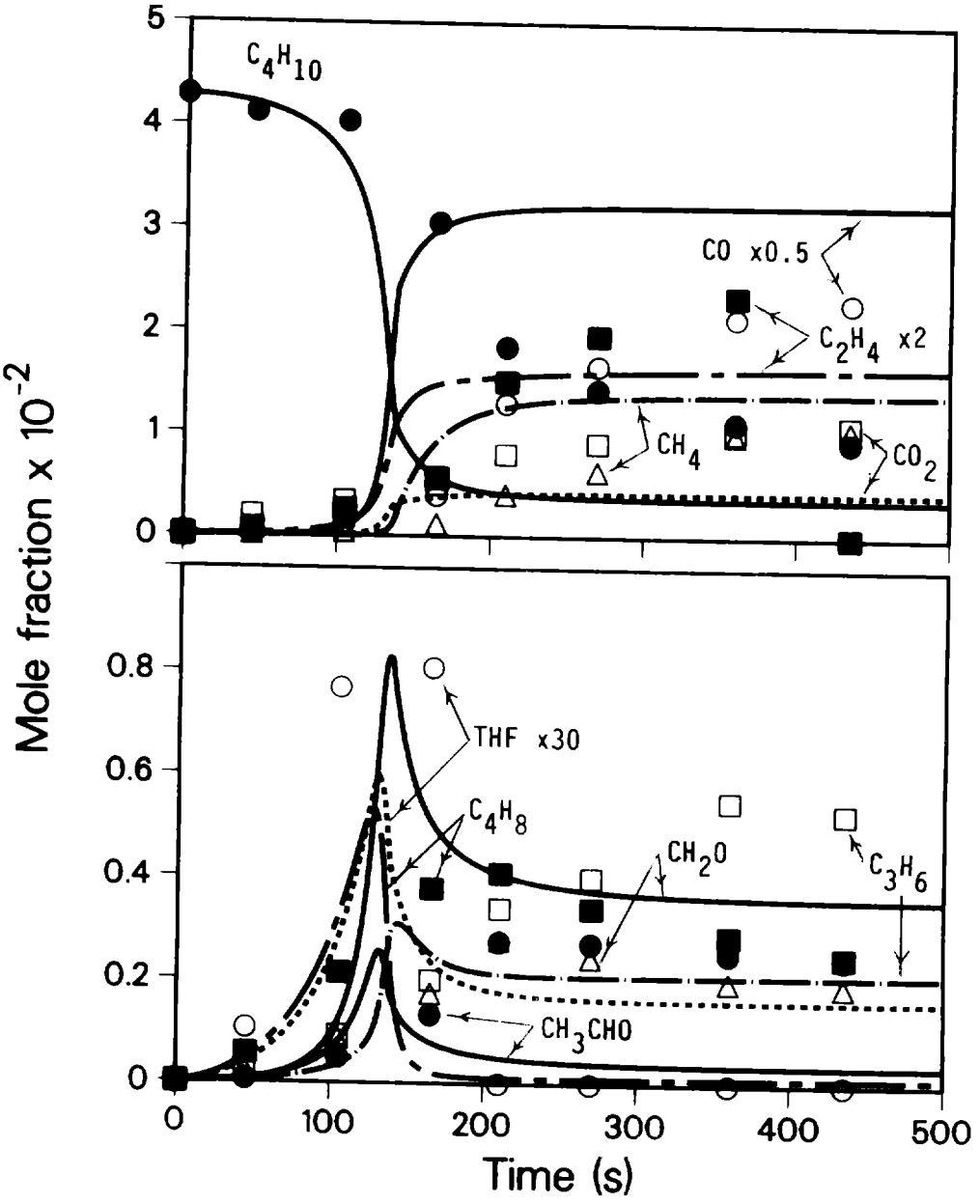
Mole fraction x 10^{-2}
C_4H_{10}
CO x0.5
C_2H_4 x2
CH_4
CO_2
THF x30
C_4H_8
CH_2O
C_3H_6
CH_3CHO
Time (s)
0
100
200
300
400
500
1
2
3
4
5
0.2
0.4
0.6
0.8

Fig. 4

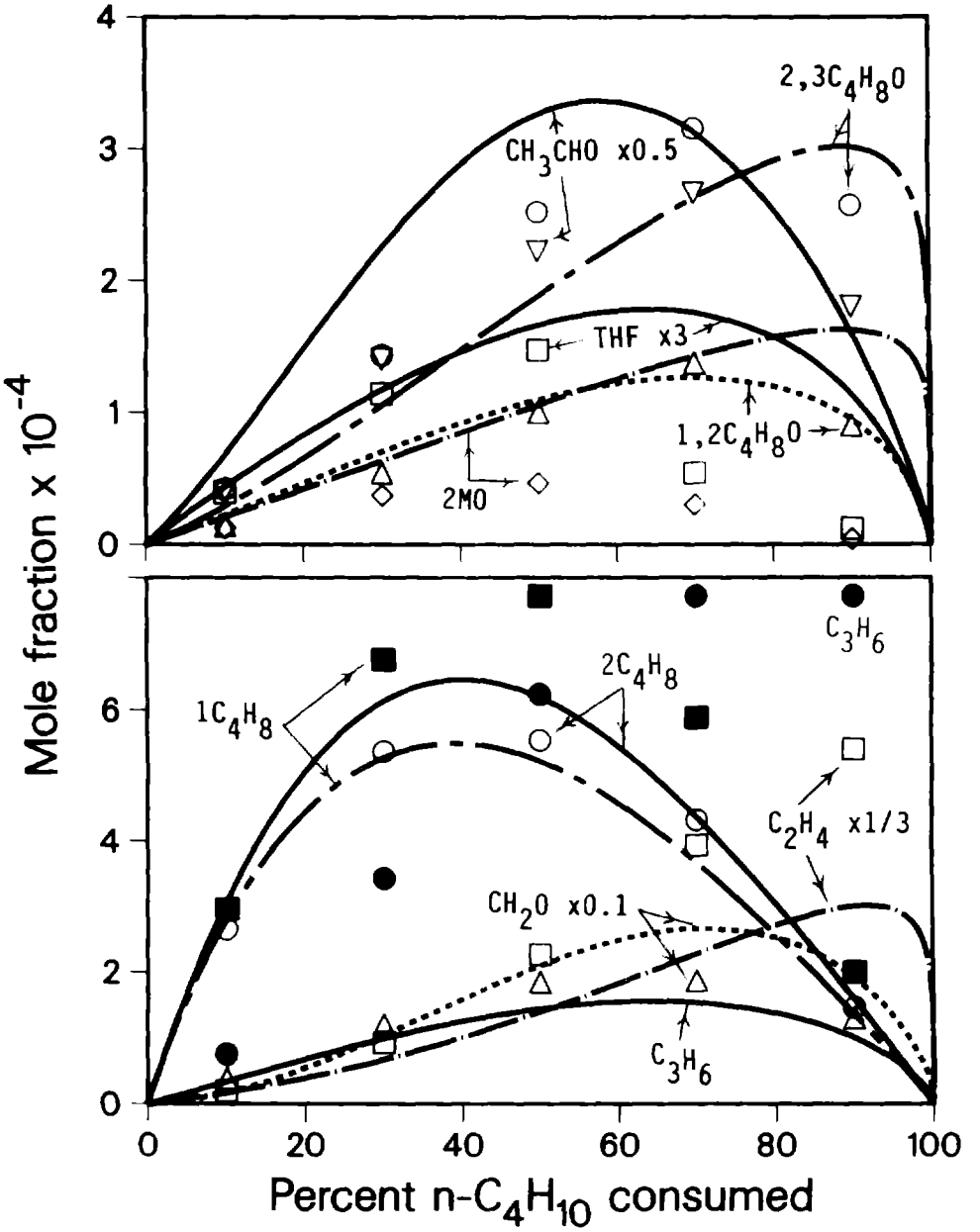
Mole fraction x 10^{-4}
Percent n-C_4H_{10} consumed
$2,3C_4H_8O$
CH_3CHO x0.5
THF x3
$1,2C_4H_8O$
2MO
C_3H_6
$2C_4H_8$
$1C_4H_8$
C_2H_4 x1/3
CH_2O x0.1
C_3H_6
0
20
40
60
80
100
0
1
2
3
4
0
2
4
6

Fig. 5

Appendix

REACTION MECHANISM FOR N-BUTANE OXIDATION

Reaction rate parameters are in cm^3-mole-sec-kcal units. Reaction rate constants are described by the three-parameter expression $k=AT^n exp(-E_a/RT)$. In the reaction mechanism, the species "M" signifies a third body. All third body efficiencies are 1.0, except for the following:

$k_{25}(H_2O)=20k_{25}(N_2)$

$k_{26}(H_2O)=21k_{26}(N_2)$; $k_{26}(CO_2)=5k_{26}(N_2)$; $k_{26}(CO)=2k_{26}(N_2)$; $k_{26}(H_2)=3.3k_{26}(N_2)$

$k_{51}(H_2O)=7k_{51}(N_2)$; $k_{51}(O_2)=0.78k_{51}(N_2)$; $k_{51}(H_2O_2)=7.7k_{51}(N_2)$

$k_{57}(H_2O)=6k_{57}(N_2)$; $k_{57}(H)=2k_{57}(N_2)$; $k_{57}(H_2)=3k_{57}(N_2)$.

Also, reactions 1, 15, 24, and 60 are described as "unimolecular" reactions in fall-off region who rate constants conform to the Lindemann form, $k=k^{\infty}/(1+\alpha/[M])$, where $\alpha=(arc)(T^{arp})exp(-arx/RT)$.

The parameters for k^{∞} are given in the main listing, and the parameters arc, arp, and arx are listed on the last page of the Appendix.

	Reaction			Forward rate A	n	Ea	Reverse rate A	n	Ea
1	ch4+m	=	ch3+h+m	6.300e+14	0.00	1.040e+05	1.279e+09	1.00	-3.920e+03
2	ch4+h	=	ch3+h2	1.250e+14	0.00	1.190e+04	4.800e+12	0.00	1.143e+04
3	ch4+oh	=	ch3+h2o	3.500e+03	3.08	2.000e+03	5.750e+02	3.08	1.668e+04
4	ch4+o	=	ch3+oh	2.130e+06	2.21	6.480e+03	3.557e+04	2.21	3.920e+03
5	c2h6+ch3	=	c2h5+ch4	5.500e-01	4.00	8.280e+03	3.000e+10	0.00	1.250e+04
6	hco+oh	=	co+h2o	1.000e+14	0.00	0.	2.800e+15	0.00	1.051e+05
7	oh+co	=	h+co2	1.500e+07	1.30	-7.650e+02	1.680e+09	1.30	2.158e+04
8	h+o2	=	oh+o	5.130e+16	-0.82	1.651e+04	1.305e+13	0.00	6.770e+02
9	h2+o	=	h+oh	3.870e+04	2.70	3.150e+03	1.785e+04	2.70	1.200e+03
10	o+h2o	=	oh+oh	6.800e+13	0.00	1.835e+04	6.300e+12	0.00	1.100e+03
11	h+h2o	=	oh+h2	9.500e+13	0.00	2.030e+04	2.200e+13	0.00	5.146e+03
12	hco+m	=	h+co+m	1.450e+14	0.00	1.900e+04	5.050e+11	1.00	1.553e+03
13	h2o2+oh	=	h2o+ho2	1.000e+13	0.00	1.800e+03	2.800e+13	0.00	3.279e+04
14	c2h4+o	=	ch3+hco	3.300e+12	0.00	1.130e+03	1.574e+11	0.00	3.118e+04
15	c2h5+m	=	c2h4+h+m	1.071e+18	-1.00	4.310e+04	2.210e+13	0.00	2.066e+03
16	ch3oh+m	=	ch3+oh+m	3.000e+18	0.00	8.000e+04	1.450e+13	1.00	-1.098e+04
17	c2h6+h	=	c2h5+h2	5.370e+02	3.50	5.200e+03	9.720e+02	3.50	2.732e+04
18	ho2+ch3oh	=	ch2oh+h2o2	6.300e+12	0.00	1.936e+04	1.000e+07	1.66	1.144e+04
19	c2h5+o2	=	c2h4+ho2	1.500e+11	0.00	0.	1.330e+11	0.00	1.370e+04
20	c2h6+oh	=	c2h5+h2o	5.125e+06	2.06	8.550e+02	1.010e+07	2.06	2.298e+04
21	c2h6+o	=	c2h5+oh	1.130e+14	0.00	7.850e+03	2.080e+13	0.00	1.272e+04
22	ch3+ho2	=	ch3o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	2.561e+04
23	co+ho2	=	co2+oh	1.510e+14	0.00	2.365e+04	1.700e+15	0.00	8.550e+04
24	c2h6	=	ch3+ch3	4.271e+19	-1.00	8.800e+04	1.670e+13	0.00	-3.060e+02
25	h2o+m	=	h+oh+m	2.200e+16	0.00	1.050e+05	1.400e+23	-2.00	0.
26	ho2+m	=	h+o2+m	2.310e+15	0.00	4.590e+04	1.650e+15	0.00	-1.000e+03
27	co2+m	=	co+o+m	5.500e+21	-1.00	1.318e+05	5.900e+15	0.00	4.100e+03
28	co2+o	=	co+o2	2.780e+12	0.00	4.383e+04	3.140e+11	0.00	3.760e+04
29	hco+h	=	co+h2	2.000e+14	0.00	0.	1.310e+15	0.00	9.000e+04
30	o+hco	=	co+oh	1.000e+14	0.00	0.	2.880e+14	0.00	8.790e+04
31	ch2o+m	=	hco+h+m	3.300e+16	0.00	8.100e+04	1.400e+11	1.00	-1.177e+04
32	ch2o+oh	=	hco+h2o	7.500e+12	0.00	1.700e+02	2.590e+12	0.00	2.999e+04
33	ch2o+h	=	hco+h2	3.300e+14	0.00	1.050e+04	2.640e+13	0.00	2.517e+04
34	ch2o+o	=	hco+oh	5.000e+13	0.00	4.600e+03	1.750e+12	0.00	1.717e+04
35	ch3+oh	=	ch2o+h2	4.000e+12	0.00	0.	1.200e+14	0.00	7.172e+04
36	ch3+o	=	ch2o+h	1.300e+14	0.00	2.000e+03	1.700e+15	0.00	7.163e+04
37	ch3+o2	=	ch3o+o	4.800e+13	0.00	2.900e+04	3.040e+14	0.00	7.330e+02
38	ch2o+ch3	=	hco+ch4	1.000e+10	0.50	6.000e+03	2.090e+10	0.50	2.114e+04
39	hco+ch3	=	ch4+co	3.000e+11	0.50	0.	5.140e+13	0.50	9.047e+04
40	ch3o+m	=	ch2o+h+m	3.888e+37	-6.65	3.326e+04	7.706e+32	-6.65	9.697e+03
41	c2h4+m	=	c2h2+h2+m	9.330e+16	0.00	7.720e+04	4.600e+12	1.00	3.652e+04
42	ho2+o	=	o2+oh	5.000e+13	0.00	1.000e+03	6.420e+13	0.00	5.661e+04
43	hco+ho2	=	ch2o+o2	1.000e+14	0.00	3.000e+03	3.660e+15	0.00	4.604e+04
44	ch3o+o2	=	ch2o+ho2	7.600e+10	0.00	2.700e+03	1.280e+11	0.00	3.217e+04
45	ch3+ho2	=	ch4+o2	1.000e+12	0.00	4.000e+02	7.630e+13	0.00	5.859e+04
46	hco+o2	=	co+ho2	3.000e+12	0.00	0.	6.730e+12	0.00	3.229e+04
47	h+ho2	=	oh+oh	2.500e+14	0.00	1.900e+03	1.200e+13	0.00	4.010e+04
48	h+ho2	=	h2+o2	2.500e+13	0.00	7.000e+02	5.500e+13	0.00	5.780e+04
49	oh+ho2	=	h2o+o2	5.000e+13	0.00	1.000e+03	6.330e+14	0.00	7.386e+04
50	h2o2+o2	=	ho2+ho2	2.955e+12	0.00	3.815e+04	3.020e+12	0.00	1.390e+03
51	h2o2+m	=	oh+oh+m	6.000e+16	0.00	4.550e+04	4.550e+14	0.00	-5.070e+03

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
52	ho2+h2	=	h2o2+h	7.300e+11	0.00	1.870e+04	1.700e+12	0.00	3.750e+03
53	ch4+ho2	=	ch3+h2o2	1.130e+13	0.00	2.046e+04	7.490e+08	0.00	1.280e+03
54	ch2o+ho2	=	hco+h2o2	2.000e+11	0.00	8.000e+03	2.200e+10	0.00	6.593e+03
55	oh+m	=	o+h+m	8.000e+19	-1.00	1.037e+05	1.000e+16	0.00	0.
56	o2+m	=	o+o+m	5.100e+15	0.00	1.150e+05	4.700e+15	-0.28	0.
57	h2+m	=	h+h+m	2.200e+14	0.00	9.600e+04	3.000e+15	0.00	0.
58	c2h4+m	=	c2h3+h+m	6.300e+18	0.00	1.087e+05	2.000e+17	0.00	0.
59	c2h5+c2h3	=	c2h4+c2h4	3.000e+12	0.00	0.	5.000e+14	0.00	6.470e+04
60	c2h3+m	=	c2h2+h+m	3.612e+16	-1.00	4.428e+04	5.540e+12	0.00	2.410e+03
61	c2h4+h	=	c2h3+h2	1.500e+07	2.00	6.000e+03	1.750e+06	2.00	5.110e+03
62	c2h4+oh	=	c2h3+h2o	2.020e+13	0.00	5.955e+03	1.015e+13	0.00	2.022e+04
63	o+c2h4	=	ch2o+ch2	2.500e+13	0.00	5.000e+03	3.016e+12	0.00	1.568e+04
64	c2h2+m	=	c2h+h+m	1.000e+14	0.00	1.140e+05	1.108e+09	1.00	7.670e+02
65	c2h2+o2	=	hco+hco	4.000e+12	0.00	2.800e+04	1.000e+11	0.00	6.365e+04
66	c2h2+h	=	c2h+h2	2.000e+14	0.00	1.900e+04	4.179e+13	0.00	1.321e+04
67	c2h2+oh	=	c2h+h2o	6.000e+12	0.00	7.000e+03	5.428e+12	0.00	1.636e+04
68	o+c2h2	=	c2h+oh	3.200e+15	-0.60	1.700e+04	2.937e+14	-0.60	9.112e+02
69	c2h2+o	=	ch2+co	6.700e+13	0.00	4.000e+03	1.260e+13	0.00	5.467e+04
70	c2h+o2	=	hco+co	1.000e+13	0.00	7.000e+03	8.444e+12	0.00	1.384e+05
71	c2h+o	=	co+ch	5.000e+13	0.00	0.	3.160e+13	0.00	5.943e+04
72	ch2+o2	=	hco+oh	1.000e+14	0.00	3.700e+03	4.117e+13	0.00	7.658e+04
73	ch2+o	=	ch+oh	1.900e+11	0.68	2.500e+04	5.863e+10	0.68	2.593e+04
74	ch2+h	=	ch+h2	2.700e+11	0.67	2.570e+04	1.897e+11	0.67	2.873e+04
75	ch2+oh	=	ch+h2o	2.700e+11	0.67	2.570e+04	8.213e+11	0.67	4.388e+04
76	ch+o2	=	co+oh	1.350e+11	0.67	2.570e+04	5.187e+11	0.67	1.856e+05
77	ch+o2	=	hco+o	1.000e+13	0.00	0.	1.334e+13	0.00	7.195e+04
78	oh+ch3oh	=	ch2oh+h2o	4.000e+12	0.00	2.000e+03	1.850e+07	1.66	2.531e+04
79	h+ch3oh	=	ch3+h2o	5.200e+12	0.00	5.340e+03	2.080e+12	0.00	3.695e+04
80	h+ch3oh	=	ch2oh+h2	3.000e+13	0.00	7.000e+03	3.210e+07	1.66	1.516e+04
81	ch3+ch3oh	=	ch4+ch2oh	1.800e+11	0.00	9.800e+03	5.040e+06	1.66	1.843e+04
82	o+ch3oh	=	ch2oh+oh	1.700e+12	0.00	2.285e+03	7.980e+05	1.66	8.347e+03
83	o2+ch2oh	=	ch2o+ho2	1.000e+12	0.00	6.000e+03	8.770e+17	-1.66	2.832e+04
84	ch2oh+m	=	ch2o+h+m	2.500e+13	0.00	2.900e+04	4.850e+16	-0.66	7.583e+03
85	c2h3+o2	=	c2h2+ho2	1.000e+12	0.00	1.000e+04	1.000e+12	0.00	1.787e+04
86	c2h4+oh	=	ch3+ch2o	2.000e+12	0.00	9.560e+02	6.000e+11	0.00	1.648e+04
87	c2h2+oh	=	ch3+co	1.200e-08	0.00	5.000e+02	2.550e-08	0.00	5.800e+04
88	ch3+ch2	=	c2h4+h	3.000e+13	0.00	0.	0.	0.00	5.895e+04
89	c3h8	=	ch3+c2h5	1.680e+16	0.00	8.484e+04	1.500e+10	1.00	-3.200e+02
90	ch3+c3h8	=	ch4+ic3h7	1.990e+11	0.00	9.600e+03	1.585e+12	0.00	1.648e+04
91	ch3+c3h8	=	ch4+nc3h7	3.980e+11	0.00	1.140e+04	5.129e+12	0.00	1.858e+04
92	h+c3h8	=	h2+ic3h7	8.775e+06	2.00	5.000e+03	7.683e+12	0.00	1.587e+04
93	h+c3h8	=	h2+nc3h7	5.628e+07	2.00	7.700e+03	9.120e+12	0.00	1.446e+04
94	ic3h7	=	h+c3h6	6.300e+13	0.00	3.690e+04	1.000e+13	0.00	1.500e+03
95	ic3h7	=	ch3+c2h4	2.000e+10	0.00	2.950e+04	4.560e+04	1.00	4.290e+03
96	nc3h7	=	ch3+c2h4	9.600e+13	0.00	3.100e+04	1.260e+11	0.00	7.700e+03
97	nc3h7	=	h+c3h6	1.250e+14	0.00	3.700e+04	7.940e+12	0.00	2.900e+03
98	ic3h7+c3h8	=	nc3h7+c3h8	3.000e+10	0.00	1.290e+04	3.000e+10	0.00	1.290e+04
99	c2h3+c3h8	=	c2h4+ic3h7	1.000e+11	0.00	1.040e+04	1.310e+11	0.00	1.780e+04
100	c2h3+c3h8	=	c2h4+nc3h7	1.000e+11	0.00	1.040e+04	1.310e+11	0.00	1.780e+04
101	c2h5+c3h8	=	c2h6+ic3h7	1.000e+11	0.00	1.040e+04	3.630e+10	0.00	9.934e+03
102	c2h5+c3h8	=	c2h6+nc3h7	1.000e+11	0.00	1.040e+04	3.630e+10	0.00	9.934e+03

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
103	c3h8+o	=	ic3h7+oh	2.810e+13	0.00	5.200e+03	1.870e+12	0.00	9.607e+03
104	c3h8+o	=	nc3h7+oh	1.130e+14	0.00	7.850e+03	7.530e+12	0.00	1.226e+04
105	c3h8+oh	=	nc3h7+h2o	1.054e+10	0.97	1.586e+03	6.931e+09	0.97	2.325e+04
106	c3h8+oh	=	ic3h7+h2o	4.670e+07	1.61	-3.500e+01	3.071e+07	1.61	2.163e+04
107	c3h8+ho2	=	ic3h7+h2o2	2.000e+12	0.00	1.700e+04	4.160e+11	0.00	7.426e+03
108	c3h8+ho2	=	nc3h7+h2o2	1.700e+13	0.00	2.046e+04	2.330e+12	0.00	9.826e+03
109	c3h6+o	=	c2h4+ch2o	6.800e+04	2.56	-1.130e+03	6.640e+04	2.56	8.054e+04
110	ic3h7+o2	=	c3h6+ho2	3.600e+10	0.00	0.	1.990e+11	0.00	1.748e+04
111	nc3h7+o2	=	c3h6+ho2	3.600e+10	0.00	0.	1.990e+11	0.00	1.748e+04
112	c3h8+o2	=	ic3h7+ho2	4.000e+13	0.00	4.750e+04	2.080e+12	0.00	0.
113	c3h8+o2	=	nc3h7+ho2	4.000e+13	0.00	4.750e+04	2.080e+12	0.00	0.
114	c3h6+oh	=	c2h5+ch2o	1.000e+11	0.00	0.	1.140e+13	0.00	1.735e+04
115	c3h6+o	=	c2h5+hco	6.800e+04	2.56	-1.130e+03	1.360e+04	2.56	2.879e+04
116	oh+c3h6	=	ch3+ch3cho	1.000e+11	0.00	0.	2.765e+11	0.00	2.040e+04
117	o+c3h6	=	ch3+ch3co	6.800e+04	2.56	-1.130e+03	1.035e+04	2.56	3.664e+04
118	ch3cho+h	=	ch3co+h2	4.000e+13	0.00	4.200e+03	1.760e+13	0.00	2.366e+04
119	ch3cho+oh	=	ch3co+h2o	1.000e+13	0.00	0.	1.900e+13	0.00	3.662e+04
120	ch3cho+o	=	ch3co+oh	5.000e+12	0.00	1.790e+03	1.000e+12	0.00	1.916e+04
121	ch3cho+ch3	=	ch3co+ch4	1.740e+12	0.00	8.440e+03	2.100e+13	0.00	2.844e+04
122	ch3cho+ho2	=	ch3co+h2o2	1.200e+12	0.00	1.070e+04	1.000e+12	0.00	1.410e+04
123	ch3cho	=	ch3+hco	7.000e+15	0.00	8.177e+04	3.800e+09	1.00	0.
124	ch3cho+o2	=	ch3co+ho2	2.000e+13	0.50	4.220e+04	1.000e+07	0.50	4.000e+03
125	ch3co+m	=	ch3+co+m	8.640e+15	0.00	1.440e+04	7.680e+10	0.00	5.970e+03
126	h+c3h6	=	c3h5+h2	5.000e+12	0.00	1.500e+03	1.500e+12	0.00	1.770e+04
127	ch3+c3h6	=	ch4+c3h5	1.600e+12	0.00	8.800e+03	1.320e+13	0.00	2.548e+04
128	c3h6+c2h5	=	c3h5+c2h6	1.000e+11	0.00	9.800e+03	7.940e+11	0.00	2.050e+04
129	c3h6+oh	=	c3h5+h2o	9.950e+12	0.00	3.062e+03	3.730e+07	0.00	7.275e+04
130	c3h8+c3h5	=	ic3h7+c3h6	2.000e+11	0.00	1.610e+04	3.980e+10	0.00	9.700e+03
131	c3h8+c3h5	=	nc3h7+c3h6	7.940e+11	0.00	2.050e+04	1.000e+11	0.00	9.800e+03
132	c3h5	=	c3h4+h	3.980e+13	0.00	7.000e+04	1.000e+13	0.00	1.500e+03
133	c3h5+o2	=	c3h4+ho2	6.000e+10	0.00	1.000e+04	1.200e+11	0.00	1.000e+04
134	1c4h8	=	c3h5+ch3	1.500e+19	-1.00	7.340e+04	1.350e+13	0.00	0.
135	1c4h8	=	c2h3+c2h5	1.000e+19	-1.00	9.677e+04	9.000e+12	0.00	0.
136	1c4h8+o	=	ch3cho+c2h4	1.300e+13	0.00	8.500e+02	2.070e+12	0.00	8.510e+04
137	1c4h8+o	=	ch3co+c2h5	1.300e+13	0.00	8.500e+02	2.350e+12	0.00	3.815e+04
138	1c4h8+oh	=	ch3cho+c2h5	1.000e+11	0.00	0.	9.330e+12	0.00	1.993e+04
139	1c4h8+oh	=	ch3co+c2h6	1.000e+11	0.00	0.	9.830e+12	0.00	3.243e+04
140	c3h4+o	=	ch2o+c2h2	1.000e+12	0.00	0.	1.080e+12	0.00	8.173e+04
141	c3h4+o	=	hco+c2h3	1.000e+12	0.00	0.	2.980e+10	0.00	3.082e+04
142	c3h4+oh	=	ch2o+c2h3	1.000e+12	0.00	0.	8.490e+11	0.00	1.824e+04
143	c3h4+oh	=	hco+c2h4	3.000e+13	0.00	0.	5.840e+11	0.00	3.381e+04
144	c3h6	=	c2h3+ch3	6.250e+15	0.00	8.580e+04	1.000e+10	1.00	0.
145	c2h2+o	=	hcco+h	3.560e+04	2.70	1.391e+03	5.030e+02	2.70	1.279e+04
146	c2h2+oh	=	ch2co+h	3.200e+11	0.00	2.000e+02	3.158e+12	0.00	2.086e+04
147	ch2co+h	=	ch3+co	1.100e+13	0.00	3.400e+03	2.400e+12	0.00	4.020e+04
148	ch2co+o	=	hco+hco	1.000e+13	0.00	2.400e+03	3.500e+11	0.00	3.350e+04
149	ch2co+oh	=	ch2o+hco	2.800e+13	0.00	0.	2.757e+13	0.00	1.850e+04
150	ch2co+m	=	ch2+co+m	2.000e+16	0.00	6.000e+04	4.610e+10	0.00	0.
151	ch2co+o	=	hcco+oh	5.000e+13	0.00	8.000e+03	7.150e+10	0.00	8.000e+03
152	ch2co+oh	=	hcco+h2o	7.500e+12	0.00	3.000e+03	1.060e+11	0.00	1.100e+04
153	ch2co+h	=	hcco+h2	7.500e+13	0.00	8.000e+03	2.450e+11	0.00	8.000e+03

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
154	hcco+oh	=	hco+h+co	1.000e+13	0.00	0.	0.	0.00	0.
155	hcco+h	=	ch2+co	1.100e+14	0.00	0.	6.660e+13	0.00	3.926e+04
156	o+hcco	=	h+co+co	1.100e+14	0.00	0.	0.	0.00	0.
157	c3h6	=	c3h5+h	6.310e+14	0.00	8.920e+04	1.000e+14	0.00	0.
158	c3h5+h	=	c3h4+h2	1.000e+13	0.00	0.	1.000e+13	0.00	4.000e+04
159	c3h5+ch3	=	c3h4+ch4	1.000e+12	0.00	0.	1.000e+13	0.00	4.000e+04
160	c4h7	=	c4h6+h	1.200e+14	0.00	4.930e+04	4.000e+13	0.00	1.300e+03
161	c4h7	=	c2h4+c2h3	1.000e+11	0.00	3.700e+04	5.000e+10	0.00	7.000e+03
162	c2h3+c2h4	=	c4h6+h	5.000e+11	0.00	7.300e+03	1.000e+13	0.00	4.700e+03
163	c2h6+o2	=	c2h5+ho2	4.000e+13	0.00	5.090e+04	3.000e+11	0.00	0.
164	c2h6+ho2	=	c2h5+h2o2	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
165	1c4h8+h	=	c4h7+h2	5.000e+13	0.00	3.900e+03	4.000e+13	0.00	2.520e+04
166	1c4h8+oh	=	nc3h7+ch2o	1.000e+11	0.00	0.	1.620e+12	0.00	1.323e+04
167	1c4h8+o	=	c3h6+ch2o	7.230e+05	2.34	-1.050e+03	2.000e+05	2.34	8.028e+04
168	1c4h8+ch3	=	c4h7+ch4	1.000e+11	0.00	7.300e+03	6.000e+11	0.00	1.786e+04
169	2c4h8+h	=	c4h7+h2	5.000e+13	0.00	3.800e+03	3.160e+13	0.00	2.230e+04
170	2c4h8+oh	=	c2h5+ch3cho	1.000e+11	0.00	0.	2.430e+13	0.00	1.993e+04
171	2c4h8+o	=	ic3h7+hco	2.790e+06	2.12	-1.775e+03	1.050e+05	2.12	2.404e+04
172	2c4h8+ch3	=	c4h7+ch4	1.000e+11	0.00	8.200e+03	6.000e+11	0.00	1.876e+04
173	c2h6+c2h4	=	c2h5+c2h5	5.000e+11	0.00	6.000e+04	5.000e+11	0.00	0.
174	1c4h8+oh	=	c4h7+h2o	2.250e+13	0.00	2.217e+03	4.772e+12	0.00	2.647e+04
175	2c4h8+oh	=	c4h7+h2o	3.900e+13	0.00	2.217e+03	4.772e+12	0.00	2.647e+04
176	c3h5+c4h7	=	c3h6+c4h6	6.310e+12	0.00	0.	1.000e+10	0.00	5.000e+04
177	1c4h8	=	h+c4h7	4.107e+18	-1.00	9.735e+04	5.000e+13	0.00	0.
178	2c4h8	=	h+c4h7	4.107e+18	-1.00	9.735e+04	5.000e+13	0.00	0.
179	c4h7+o2	=	c4h6+ho2	0.	0.00	0.	0.	0.00	1.700e+04
180	h+c4h7	=	c4h6+h2	3.160e+13	0.00	0.	1.066e+13	0.00	5.681e+04
181	1c5h10	=	c2h5+c3h5	1.000e+16	0.00	7.140e+04	1.000e+13	0.00	0.
182	c2h5+c4h7	=	c4h6+c2h6	3.980e+12	0.00	0.	3.211e+12	0.00	4.984e+04
183	c2h5+c4h7	=	c2h4+1c4h8	5.000e+11	0.00	0.	8.478e+11	0.00	5.633e+04
184	c2h5+c4h7	=	c2h4+2c4h8	5.000e+11	0.00	0.	8.478e+11	0.00	5.633e+04
185	c2h3+c4h7	=	c2h4+c4h6	3.980e+12	0.00	0.	1.157e+13	0.00	5.771e+04
186	c4h6	=	c2h3+c2h3	4.027e+19	-1.00	9.815e+04	1.260e+13	0.00	0.
187	c4h6+oh	=	c2h5+ch2co	1.000e+12	0.00	0.	3.730e+12	0.00	3.002e+04
188	c4h6+oh	=	ch2o+c3h5	1.000e+12	0.00	0.	3.501e+06	0.00	7.106e+04
189	c4h6+oh	=	c2h3+ch3cho	1.000e+12	0.00	0	5.437e+11	0.00	1.855e+04
190	c4h6+o	=	c2h4+ch2co	1.000e+12	0.00	0	6.377e+11	0.00	9.434e+04
191	c4h6+o	=	ch2o+c3h4	1.000e+12	0.00	0	1.075e+12	0.00	7.905e+04
192	1c5h10+o	=	c5h9+oh	2.540e+05	2.56	-1.130e+03	7.000e+11	0.00	2.990e+04
193	2c5h10+o	=	c5h9+oh	2.430e+05	2.56	-1.130e+03	7.000e+11	0.00	2.990e+04
194	1c5h10+o	=	1c4h8+ch2o	1.000e+10	0.00	0.	6.000e+13	0.00	8.670e+04
195	2c5h10+o	=	c3h6+ch3cho	1.000e+10	0.00	0.	1.000e+12	0.00	8.100e+04
196	ch3+c2h3	=	ch4+c2h2	7.940e+11	0.00	0.	7.557e+13	0.00	6.605e+04
197	ch3+c2h5	=	ch4+c2h4	7.940e+11	0.00	0.	8.075e+12	0.00	6.689e+04
198	c2h5+c3h5	=	c3h6+c2h4	1.260e+12	0.00	0.	1.000e+10	0.00	5.000e+04
199	2c4h8+o	=	c2h4+ch3cho	4.640e+05	2.12	-1.775e+03	7.400e+04	2.12	8.248e+04
200	ch3oh+ch2o	=	ch3o+ch3o	1.533e+12	0.00	7.957e+04	3.000e+13	0.00	0.
201	ch2o+ch3o	=	ch3oh+hco	1.150e+11	0.00	1.280e+03	3.020e+11	0.00	1.816e+04
202	ch4+ch3o	=	ch3+ch3oh	2.000e+11	0.00	7.000e+03	1.046e+09	0.00	5.000e+04
203	c2h6+ch3o	=	c2h5+ch3oh	3.000e+11	0.00	7.000e+03	1.714e+10	0.00	5.000e+04
204	c2h3+h	=	c2h2+h2	2.000e+13	0.00	2.500e+03	1.331e+13	0.00	6.808e+04

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
205	c3h8+ch3o	=	nc3h7+ch3oh	3.000e+11	0.00	7.000e+03	1.220e+10	0.00	9.182e+03
206	c3h8+ch3o	=	ic3h7+ch3oh	3.000e+11	0.00	7.000e+03	1.220e+10	0.00	9.182e+03
207	ch3o+ch3oh	=	ch2oh+ch3oh	1.510e+12	0.00	7.000e+03	2.190e+05	1.66	1.085e+04
208	ch3o+ch3cho	=	ch3oh+ch3co	1.150e+11	0.00	1.280e+03	3.000e+11	0.00	1.816e+04
209	ch3oh+oh	=	ch3o+h2o	1.230e+13	0.00	3.250e+03	3.168e+13	0.00	2.146e+04
210	c2h5+h	=	ch3+ch3	3.160e+13	0.00	0.	5.000e+10	0.00	7.400e+03
211	1c5h10+oh	=	c5h9+h2o	6.800e+13	0.00	3.060e+03	5.000e+12	0.00	2.650e+04
212	2c5h10+oh	=	c5h9+h2o	4.300e+13	0.00	3.060e+03	5.000e+12	0.00	2.650e+04
213	2c5h10+oh	=	nc3h7+ch3cho	2.000e+10	0.00	-4.000e+03	2.000e+13	0.00	2.000e+04
214	1c5h10+h	=	c5h9+h2	2.800e+13	0.00	4.000e+03	1.000e+12	0.00	1.400e+04
215	2c5h10+h	=	c5h9+h2	2.900e+13	0.00	4.000e+03	1.000e+12	0.00	1.400e+04
216	1c5h10+ch3	=	c5h9+ch4	1.000e+11	0.00	7.300e+03	6.000e+11	0.00	1.790e+04
217	2c5h10+ch3	=	c5h9+ch4	1.000e+11	0.00	8.200e+03	6.000e+11	0.00	1.880e+04
218	c5h9	=	c3h5+c2h4	2.500e+13	0.00	3.000e+04	1.500e+10	0.00	7.400e+03
219	c5h9	=	c2h3+c3h6	2.500e+13	0.00	3.000e+04	1.500e+10	0.00	7.400e+03
220	2c5h10	=	ch3+c4h7	5.000e+06	0.00	7.300e+04	2.500e+13	0.00	0.
221	c2h3+o2	=	ch2o+hco	8.000e+12	0.00	-2.500e+02	7.799e+12	0.00	8.630e+04
222	c2h6	=	c2h5+h	1.350e+18	-1.00	1.005e+05	3.000e+13	0.00	0.
223	c3h4+oh	=	ch2co+ch3	2.500e+12	0.00	0.	8.490e+11	0.00	1.824e+04
224	c3h8	=	nc3h7+h	1.000e+15	0.00	9.790e+04	1.000e+14	0.00	0.
225	c3h8	=	ic3h7+h	1.000e+15	0.00	9.590e+04	1.000e+14	0.00	0.
226	ch3coch3	=	ch3co+ch3	8.000e+16	0.00	8.510e+04	1.000e+12	0.00	0.
227	ch3coch3+o2	=	ch3coch2+ho2	1.200e+14	0.00	4.600e+04	2.000e+12	0.00	2.000e+03
228	ch3coch3+oh	=	ch3coch2+h2o	1.054e+10	0.97	1.586e+03	6.931e+09	0.97	2.325e+04
229	ch3coch3+h	=	ch3coch2+h2	5.628e+07	2.00	7.700e+03	9.000e+12	0.00	1.450e+05
230	ch3coch3+o	=	ch3coch2+oh	1.130e+14	0.00	7.850e+03	7.500e+12	0.00	1.230e+04
231	ch3coch3+ch3	=	ch3coch2+ch4	1.000e+12	0.00	1.150e+04	4.000e+12	0.00	1.850e+04
232	ch3coch3+ch3o	=	ch3coch2+ch3oh	1.000e+11	0.00	7.000e+03	1.000e+10	0.00	9.000e+03
233	ch3coch3+ho2	=	ch3coch2+h2o2	1.700e+13	0.00	2.046e+04	1.000e+11	0.00	8.000e+03
234	ch3coch2	=	ch2co+ch3	1.000e+14	0.00	3.100e+04	1.000e+11	0.00	6.000e+03
235	c2h5oh+m	=	ch2oh+ch3+m	3.000e+18	0.00	7.547e+04	2.270e+06	2.66	-1.375e+04
236	c2h5oh+m	=	c2h5+oh+m	3.000e+18	0.00	8.000e+04	1.096e+13	1.00	-1.309e+04
237	c2h5oh+o2	=	pc2h4oh+ho2	4.000e+13	0.00	5.090e+04	1.315e+13	0.00	1.549e+04
238	c2h5oh+o2	=	sc2h4oh+ho2	2.700e+13	0.00	4.990e+04	8.878e+12	0.00	1.449e+04
239	c2h5oh+oh	=	pc2h4oh+h2o	4.000e+12	0.00	2.000e+03	1.013e+13	0.00	3.771e+04
240	c2h5oh+oh	=	sc2h4oh+h2o	2.700e+12	0.00	0.	6.838e+12	0.00	3.572e+04
241	c2h5oh+h	=	pc2h4oh+h2	3.000e+13	0.00	7.000e+03	1.755e+13	0.00	2.756e+04
242	c2h5oh+h	=	sc2h4oh+h2	2.000e+13	0.00	3.000e+03	1.170e+13	0.00	2.356e+04
243	c2h5oh+h	=	c2h5+h2o	5.000e+12	0.00	5.300e+03	1.491e+12	0.00	3.481e+04
244	c2h5oh+o	=	pc2h4oh+oh	1.700e+12	0.00	2.285e+03	4.367e+11	0.00	2.075e+04
245	c2h5oh+o	=	sc2h4oh+oh	1.100e+12	0.00	0.	2.826e+11	0.00	1.846e+04
246	c2h5oh+ch3	=	pc2h4oh+ch4	1.800e+11	0.00	9.800e+03	2.750e+12	0.00	3.084e+04
247	c2h5oh+ch3	=	sc2h4oh+ch4	1.200e+11	0.00	6.800e+03	1.834e+12	0.00	2.784e+04
248	c2h5oh+c2h5	=	pc2h4oh+c2h6	5.000e+10	0.00	1.340e+04	6.995e+10	0.00	2.699e+04
249	c2h5oh+c2h5	=	sc2h4oh+c2h6	5.000e+10	0.00	1.040e+04	6.995e+10	0.00	2.399e+00
250	c2h5oh+ho2	=	pc2h4oh+h2o2	6.300e+12	0.00	1.936e+04	3.061e+12	0.00	2.210e+04
251	c2h5oh+ho2	=	sc2h4oh+h2o2	4.200e+12	0.00	1.500e+04	2.040e+12	0.00	1.774e+04
252	pc2h4oh	=	c2h4+oh	9.600e+13	0.00	3.400e+04	1.000e+11	0.00	0.
253	sc2h4oh+m	=	ch3cho+h+m	2.500e+13	0.00	2.901e+04	1.000e+12	0.00	5.000e+04
254	sc2h4oh+o2	=	ch3cho+ho2	1.000e+12	0.00	6.000e+03	1.000e+12	0.00	5.000e+04
255	c2h5cho	=	c2h5+hco	7.000e+15	0.00	8.500e+04	1.000e+11	0.00	0.

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
256	c2h5cho+o2	=	c2h5co+ho2	2.000e+13	0.50	4.220e+04	1.909e+14	0.50	3.090e+03
257	c2h5cho+h	=	c2h5co+h2	3.980e+13	0.00	4.200e+03	1.778e+13	0.00	2.367e+04
258	c2h5cho+oh	=	c2h5co+h2o	1.000e+13	0.00	0.	1.906e+13	0.00	3.662e+04
259	c2h5cho+o	=	c2h5co+oh	5.010e+12	0.00	1.790e+03	1.000e+12	0.00	1.916e+04
260	c2h5cho+ho2	=	c2h5co+h2o2	1.000e+12	0.00	1.100e+04	1.000e+12	0.00	1.400e+04
261	c2h5cho+ch3	=	c2h5co+ch4	7.586e+11	0.00	8.000e+03	1.514e+13	0.00	2.800e+04
262	c2h5cho+c2h5	=	c2h5co+c2h6	1.000e+12	0.00	8.000e+03	1.585e+13	0.00	2.800e+04
263	c2h5cho+nc3h7	=	c2h5co+c3h8	1.700e+12	0.00	8.440e+03	1.900e+14	0.00	1.879e+04
264	c2h5cho+ic3h7	=	c2h5co+c3h8	1.700e+12	0.00	8.440e+03	1.900e+14	0.00	1.879e+04
265	c2h5cho+c2h3	=	c2h5co+c2h4	1.700e+12	0.00	8.440e+03	2.488e+14	0.00	2.619e+04
266	c2h5cho+c3h5	=	c2h5co+c3h6	1.700e+12	0.00	8.440e+03	1.000e+13	0.00	2.800e+04
267	c2h5cho+c4h7	=	c2h5co+c4h8	1.700e+12	0.00	8.440e+03	1.000e+13	0.00	2.800e+04
268	c2h5cho+nc3h7o2	=	c2h5co+nc3h7o2h	2.000e+11	0.00	9.500e+03	5.000e+09	0.00	1.000e+04
269	c2h5cho+ch3o	=	c2h5co+ch3oh	1.000e+12	0.00	3.300e+03	3.160e+11	0.00	1.800e+04
270	c2h5cho+c2h5o	=	c2h5co+c2h5oh	6.026e+11	0.00	3.300e+03	3.020e+11	0.00	1.816e+04
271	c2h5cho+pc4h9	=	c2h5co+c4h10	1.700e+12	0.00	8.440e+03	9.695e+13	0.00	1.882e+04
272	c2h5cho+sc4h9	=	c2h5co+c4h10	1.700e+12	0.00	8.440e+03	9.695e+13	0.00	1.882e+04
273	c2h5cho+ch3o2	=	c2h5co+ch3o2h	1.000e+12	0.00	9.530e+03	2.510e+10	0.00	1.010e+04
274	c2h5cho+c2h5o2	=	c2h5co+c2h5o2h	1.290e+11	0.00	9.000e+03	2.510e+10	0.00	1.010e+04
275	c2h5cho+nc3h7o2	=	c2h5co+nc3h7o2h	2.000e+11	0.00	9.500e+03	5.000e+09	0.00	1.000e+04
276	c2h5cho+ic3h7o2	=	c2h5co+ic3h7o2h	2.000e+11	0.00	9.500e+03	5.000e+09	0.00	1.000e+04
277	c2h5cho+pc4h9o2	=	c2h5co+pc4h9o2h	2.000e+11	0.00	9.500e+03	5.000e+09	0.00	1.000e+04
278	c2h5cho+sc4h9o2	=	c2h5co+sc4h9o2h	2.000e+11	0.00	9.500e+03	5.000e+09	0.00	1.000e+04
279	c2h5cho+ch3co3	=	c2h5co+ch3co3h	1.000e+12	0.00	7.580e+03	2.000e+10	0.00	1.000e+04
280	c2h5cho+c2h5co3	=	c2h5co+c2h5co3h	1.000e+12	0.00	7.580e+03	1.995e+10	0.00	1.000e+04
281	c2h3cho+h	=	c2h3co+h2	3.980e+13	0.00	4.200e+03	1.780e+13	0.00	2.367e+04
282	c2h3cho+o	=	c2h3co+oh	5.010e+12	0.00	1.790e+03	1.000e+12	0.00	1.916e+04
283	c2h3cho+oh	=	c2h3co+h2o	1.000e+13	0.00	0.	1.906e+13	0.00	3.662e+04
284	c2h3cho+ho2	=	c2h3co+h2o2	1.700e+12	0.00	1.070e+04	1.000e+12	0.00	1.410e+04
285	c2h3cho+ch3	=	c2h3co+ch4	1.740e+12	0.00	8.440e+03	1.510e+13	0.00	2.800e+04
286	c2h3cho+c2h3	=	c2h3co+c2h4	1.740e+12	0.00	8.440e+03	1.000e+13	0.00	2.800e+04
287	c2h3cho+ch3o	=	c2h3co+ch3oh	6.026e+11	0.00	3.300e+03	3.020e+11	0.00	1.816e+04
288	c2h3cho+ch3o2	=	c2h3co+ch3o2h	1.000e+12	0.00	9.530e+03	2.510e+10	0.00	1.010e+04
289	c2h3cho+c3h5	=	c2h3co+c3h6	1.000e+12	0.00	8.000e+03	1.000e+13	0.00	2.800e+04
290	c2h3cho+c3h5o2	=	c2h3co+c3h5ooh	1.000e+12	0.00	9.500e+03	2.510e+10	0.00	1.010e+04
291	c2h3cho+c2h5	=	c2h3co+c2h6	1.740e+12	0.00	8.440e+03	1.000e+13	0.00	2.800e+04
292	c2h3cho+c2h5o	=	c2h3co+c2h5oh	1.000e+12	0.00	3.300e+03	3.020e+11	0.00	1.800e+04
293	c2h3cho+c2h5o2	=	c2h3co+c2h5o2h	1.000e+12	0.00	9.500e+03	2.510e+10	0.00	1.010e+04
294	c2h3cho+ic3h7	=	c2h3co+c3h8	1.000e+12	0.00	8.000e+03	1.000e+13	0.00	2.800e+04
295	c2h3cho+nc3h7	=	c2h3co+c3h8	1.000e+12	0.00	8.000e+03	1.000e+13	0.00	2.800e+04
296	c2h3cho+nc3h7o2	=	c2h3co+nc3h7o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
297	c2h3cho+ic3h7o2	=	c2h3co+ic3h7o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
298	c2h3cho+pc4h9o2	=	c2h3co+pc4h9o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
299	c2h3cho+sc4h9o2	=	c2h3co+sc4h9o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
300	c2h3cho+ch3co3	=	c2h3co+ch3co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
301	c2h3cho+c2h3co3	=	c2h3co+c2h3co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
302	c2h3cho+c2h5co3	=	c2h3co+c2h5co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
303	c3h6+ho2	=	c3h6o+oh	1.290e+12	0.00	1.490e+04	1.000e-10	0.00	0.
304	c3h6o+m	=	c2h4+ch2o+m	6.000e+14	0.00	6.000e+04	2.970e+11	1.00	3.108e+04
305	c3h6o+oh	=	c3h5o-c+h2o	1.000e+12	0.00	0.	1.000e-10	0.00	0.
306	c3h6o+h	=	c3h5o-c+h2	5.000e+12	0.00	1.500e+03	1.000e+12	0.00	2.000e+04

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
307	c3h6o+o	=	c3h5o-c+oh	3.000e+13	0.00	5.200e+03	2.000e+12	0.00	1.000e+04
308	c3h6o+ch3	=	c3h5o-c+ch4	1.600e+12	0.00	8.800e+03	7.000e+12	0.00	2.500e+04
309	c3h6o+ho2	=	c3h5o-c+h2o2	7.000e+11	0.00	1.711e+04	1.000e+11	0.00	1.500e+04
310	c3h6o+c3h5	=	c3h5o-c+c3h6	8.000e+10	0.00	1.240e+04	1.000e+11	0.00	1.500e+04
311	c3h6o+c2h3	=	c3h5o-c+c2h4	3.000e+12	0.00	1.450e+04	1.000e+11	0.00	1.500e+04
312	c3h5o-c	=	ch2choch2	1.000e+11	0.00	1.000e+04	1.000e+10	0.00	5.000e+04
313	ch2choch2	=	c2h3+ch2o	1.000e+14	0.00	3.000e+04	1.000e+10	0.00	5.000e+04
314	c3h6o+ch3o2	=	c3h5o-c+ch3o2h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	8.000e+03
315	c3h6o+c3h5o2	=	c3h5o-c+c3h5ooh	1.000e+11	0.00	8.000e+03	5.200e+09	0.00	8.000e+03
316	nc3h7o2	=	nc3h7+o2	2.530e+17	-1.00	3.320e+04	3.400e+11	0.00	-2.000e+03
317	ic3h7o2	=	ic3h7+o2	1.490e+18	-1.00	3.502e+04	3.400e+11	0.00	-2.000e+03
318	pc4h9o2	=	pc4h9+o2	2.530e+17	-1.00	3.320e+04	3.400e+11	0.00	-2.000e+03
319	sc4h9o2	=	sc4h9+o2	1.490e+18	-1.00	3.502e+04	3.400e+11	0.00	-2.000e+03
320	c2h5o2	=	c2h5+o2	7.440e+17	-1.00	3.520e+04	1.000e+12	0.00	0.
321	ch3o2	=	ch3+o2	2.015e+20	-1.00	2.980e+04	7.050e+15	0.00	-1.100e+03
322	ch3co3	=	ch3co+o2	2.900e+16	-1.00	3.730e+04	1.000e+10	0.00	-2.700e+03
323	c2h5co3	=	c2h5co+o2	2.900e+16	-1.00	3.730e+04	1.000e+10	0.00	-2.700e+03
324	c2h3co3	=	c2h3co+o2	2.900e+16	-1.00	3.730e+04	1.000e+10	0.00	-2.700e+03
325	c3h5o2	=	c3h5+o2	3.460e+14	-1.00	1.590e+04	1.200e+10	0.00	-2.300e+03
326	ch3o2h	=	ch3o+oh	6.460e+14	0.00	4.300e+04	1.000e+11	0.00	0.
327	c2h5o2h	=	c2h5o+oh	6.460e+14	0.00	4.300e+04	1.000e+11	0.00	0.
328	nc3h7o2h	=	nc3h7o+oh	8.400e+14	0.00	4.300e+04	1.000e+11	0.00	0.
329	ic3h7o2h	=	ic3h7o+oh	8.400e+14	0.00	4.300e+04	1.000e+11	0.00	0.
330	pc4h9o2h	=	pc4h9o+oh	8.400e+14	0.00	4.000e+04	1.000e+11	0.00	0.
331	sc4h9o2h	=	sc4h9o+oh	8.400e+14	0.00	4.000e+04	1.000e+11	0.00	0.
332	ch3co3h	=	ch3co2+oh	4.000e+15	0.00	4.000e+04	1.000e+11	0.00	0.
333	c2h5co3h	=	c2h5co2+oh	4.000e+15	0.00	4.000e+04	1.000e+11	0.00	0.
334	c2h3co3h	=	c2h3co2+oh	4.000e+15	0.00	4.000e+04	1.000e+11	0.00	0.
335	c3h5ooh	=	c3h5o+oh	4.000e+15	0.00	4.300e+04	1.000e+11	0.00	0.
336	c2h5o	=	ch3+ch2o	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
337	nc3h7o	=	c2h5+ch2o	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
338	nc3h7o	=	c2h5cho+h	2.510e+14	0.00	2.340e+04	1.000e+12	0.00	0.
339	ic3h7o	=	ch3+ch3cho	3.980e+14	0.00	1.720e+04	1.000e+07	1.00	1.360e+04
340	pc4h9o	=	nc3h7+ch2o	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
341	sc4h9o	=	ch3+c2h5cho	7.900e+14	0.00	1.900e+04	5.204e+08	1.00	4.049e+04
342	sc4h9o	=	c2h5+ch3cho	7.940e+14	0.00	1.530e+04	1.000e+07	0.00	1.360e+04
343	c3h5o	=	c2h3cho+h	1.000e+14	0.00	1.500e+04	1.000e+08	0.00	1.000e+04
344	c3h5o	=	c2h3+ch2o	1.000e+14	0.00	2.160e+04	1.000e+11	0.00	9.000e+03
345	c3h5o+o2	=	c2h3cho+ho2	1.000e+12	0.00	6.000e+03	1.288e+11	0.00	3.200e+04
346	ch3co2+m	=	ch3+co2+m	4.400e+15	0.00	1.050e+04	1.000e+10	0.00	5.000e+04
347	c2h5co2+m	=	c2h5+co2+m	4.400e+15	0.00	1.050e+04	1.000e+10	0.00	5.000e+04
348	c2h3co2	=	c2h3+co2	1.000e+13	0.00	1.000e+04	1.000e+10	0.00	5.000e+04
349	c2h5o+o2	=	ch3cho+ho2	1.810e+11	0.00	1.840e+03	4.630e+09	0.00	3.001e+04
350	nc3h7o+o2	=	c2h5cho+ho2	1.750e+11	0.00	1.750e+03	1.288e+11	0.00	3.217e+04
351	sc4h9o2+c4h10	=	sc4h9o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
352	sc4h9o2+c4h10	=	sc4h9o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
353	pc4h9o2+c4h10	=	pc4h9o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
354	pc4h9o2+c4h10	=	pc4h9o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
355	ic3h7o2+c4h10	=	ic3h7o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
356	ic3h7o2+c4h10	=	ic3h7o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
357	nc3h7o2+c4h10	=	nc3h7o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
358	nc3h7o2+c4h10	=	nc3h7o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
359	c2h5o2+c4h10	=	c2h5o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
360	c2h5o2+c4h10	=	c2h5o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
361	ch3o2+c4h10	=	ch3o2h+pc4h9	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
362	ch3o2+c4h10	=	ch3o2h+sc4h9	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
363	c4h10+ch3co3	=	pc4h9+ch3co3h	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
364	c4h10+ch3co3	=	sc4h9+ch3co3h	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
365	c4h10+c2h5co3	=	pc4h9+c2h5co3h	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
366	c4h10+c2h5co3	=	sc4h9+c2h5co3h	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
367	c4h10+c2h3co3	=	pc4h9+c2h3co3h	1.700e+13	0.00	2.046e+04	1.000e+12	0.00	8.000e+03
368	c4h10+c2h3co3	=	sc4h9+c2h3co3h	4.000e+12	0.00	1.700e+04	1.000e+12	0.00	8.000e+03
369	c4h10+c3h5o2	=	pc4h9+c3h5ooh	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
370	c4h10+c3h5o2	=	sc4h9+c3h5ooh	4.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
371	sc4h9o2+c3h8	=	sc4h9o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
372	sc4h9o2+c3h8	=	sc4h9o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
373	pc4h9o2+c3h8	=	pc4h9o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
374	pc4h9o2+c3h8	=	pc4h9o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
375	ic3h7o2+c3h8	=	ic3h7o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
376	ic3h7o2+c3h8	=	ic3h7o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
377	nc3h7o2+c3h8	=	nc3h7o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
378	nc3h7o2+c3h8	=	nc3h7o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
379	c2h5o2+c3h8	=	c2h5o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
380	c2h5o2+c3h8	=	c2h5o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
381	ch3o2+c3h8	=	ch3o2h+nc3h7	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
382	ch3o2+c3h8	=	ch3o2h+ic3h7	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
383	c3h8+ch3co3	=	ic3h7+ch3co3h	2.000e+12	0.00	1.700e+04	2.000e+10	0.00	1.000e+04
384	c3h8+ch3co3	=	nc3h7+ch3co3h	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
385	c3h8+c2h5co3	=	nc3h7+c2h5co3h	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
386	c3h8+c2h5co3	=	ic3h7+c2h5co3h	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
387	c3h8+c2h3co3	=	nc3h7+c2h3co3h	1.700e+13	0.00	2.046e+04	1.000e+12	0.00	8.000e+03
388	c3h8+c2h3co3	=	ic3h7+c2h3co3h	2.000e+12	0.00	1.700e+04	1.000e+12	0.00	8.000e+03
389	c3h8+c3h5o2	=	nc3h7+c3h5ooh	1.700e+13	0.00	2.046e+04	5.000e+11	0.00	6.500e+03
390	c3h8+c3h5o2	=	ic3h7+c3h5ooh	2.000e+12	0.00	1.700e+04	5.000e+11	0.00	6.500e+03
391	ch3o2+ch2o	=	ch3o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
392	c2h5o2+ch2o	=	c2h5o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
393	nc3h7o2+ch2o	=	nc3h7o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
394	ic3h7o2+ch2o	=	ic3h7o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
395	pc4h9o2+ch2o	=	pc4h9o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
396	sc4h9o2+ch2o	=	sc4h9o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
397	pc4h9o2+ch2o	=	pc4h9o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
398	sc4h9o2+ch2o	=	sc4h9o2h+hco	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
399	ch2o+ch3co3	=	hco+ch3co3h	1.000e+12	0.00	1.056e+04	1.000e+11	0.00	1.000e+04
400	ch2o+c2h5co3	=	hco+c2h5co3h	1.000e+12	0.00	7.580e+03	1.000e+10	0.00	1.000e+04
401	ch2o+c2h3co3	=	hco+c2h3co3h	1.000e+12	0.00	1.056e+04	1.000e+11	0.00	1.000e+04
402	ch3o2+ch3cho	=	ch3o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
403	c2h5o2+ch3cho	=	c2h5o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
404	nc3h7o2+ch3cho	=	nc3h7o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
405	ic3h7o2+ch3cho	=	ic3h7o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
406	pc4h9o2+ch3cho	=	pc4h9o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
407	sc4h9o2+ch3cho	=	sc4h9o2h+ch3co	3.570e+09	0.00	5.050e+03	5.000e+09	0.00	1.010e+04
408	ch3cho+ch3co3	=	ch3co+ch3co3h	1.000e+12	0.00	7.580e+03	2.000e+10	0.00	1.000e+04

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
409	ch3cho+c2h5co3	=	ch3co+c2h5co3h	1.000e+12	0.00	7.580e+03	1.000e+10	0.00	1.000e+04
410	ch3cho+c2h3co3	=	ch3co+c2h3co3h	1.000e+12	0.00	9.000e+03	6.000e+11	0.00	1.240e+04
411	ch3cho+c3h5o2	=	ch3co+c3h5ooh	1.300e+11	0.00	9.000e+03	2.500e+10	0.00	1.010e+04
412	c2h4+ch3o2	=	c2h3+ch3o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
413	c2h4+c2h5o2	=	c2h3+c2h5o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
414	c2h4+nc3h7o2	=	c2h3+nc3h7o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
415	c2h4+ic3h7o2	=	c2h3+ic3h7o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
416	c2h4+pc4h9o2	=	c2h3+pc4h9o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
417	c2h4+sc4h9o2	=	c2h3+sc4h9o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
418	c2h4+ch3co3	=	c2h3+ch3co3h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	1.000e+04
419	c2h4+c2h5co3	=	c2h3+c2h5co3h	1.000e+11	0.00	8.000e+03	1.000e+11	0.00	1.000e+04
420	c2h4+c2h3co3	=	c2h3+c2h3co3h	7.000e+11	0.00	1.711e+04	1.000e+11	0.00	1.000e+04
421	c3h6+ch3o2	=	c3h5+ch3o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
422	c3h6+c2h5o2	=	c3h5+c2h5o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
423	c3h6+nc3h7o2	=	c3h5+nc3h7o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
424	c3h6+ic3h7o2	=	c3h5+ic3h7o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
425	c3h6+pc4h9o2	=	c3h5+pc4h9o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
426	c3h6+sc4h9o2	=	c3h5+sc4h9o2h	2.000e+11	0.00	6.000e+03	2.000e+10	0.00	8.000e+03
427	c3h6+ch3co3	=	c3h5+ch3co3h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	1.000e+04
428	c3h6+c2h5co3	=	c3h5+c2h5co3h	1.000e+11	0.00	8.000e+03	1.000e+11	0.00	1.000e+04
429	c3h6+c2h3co3	=	c3h5+c2h3co3h	1.000e+13	0.00	2.000e+04	1.000e+12	0.00	8.000e+03
430	c3h5o2+c3h6	=	c3h5ooh+c3h5	3.200e+11	0.00	1.650e+04	2.600e+10	0.00	8.000e+03
431	1c4h8+c3h5o2	=	c4h7+c3h5ooh	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	8.000e+03
432	1c4h8+ch3co3	=	c4h7+ch3co3h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	1.000e+04
433	1c4h8+c2h5co3	=	c4h7+c2h5co3h	1.000e+11	0.00	8.000e+03	1.000e+11	0.00	1.000e+04
434	2c4h8+c3h5o2	=	c4h7+c3h5ooh	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	8.000e+03
435	2c4h8+ch3co3	=	c4h7+ch3co3h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	1.000e+04
436	2c4h8+c2h5co3	=	c4h7+c2h5co3h	1.000e+11	0.00	8.000e+03	1.000e+11	0.00	1.000e+04
437	c3h6o+ch3o2	=	c3h5o-c+ch3o2h	1.000e+11	0.00	8.000e+03	2.000e+10	0.00	8.000e+03
438	c3h6o+c3h5o2	=	c3h5o-c+c3h5ooh	1.000e+11	0.00	8.000e+03	5.200e+09	0.00	8.000e+03
439	ch4+ch3o2	=	ch3+ch3o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
440	ch4+c2h5o2	=	ch3+c2h5o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
441	ch4+nc3h7o2	=	ch3+nc3h7o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
442	ch4+ic3h7o2	=	ch3+ic3h7o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
443	ch4+pc4h9o2	=	ch3+pc4h9o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
444	ch4+sc4h9o2	=	ch3+sc4h9o2h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
445	ch4+ch3co3	=	ch3+ch3co3h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
446	ch4+c2h5co3	=	ch3+c2h5co3h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
447	ch4+c2h3co3	=	ch3+c2h3co3h	1.130e+13	0.00	2.046e+04	7.500e+08	0.00	1.280e+03
448	ch3oh+ch3o2	=	ch2oh+ch3o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
449	ch3oh+c2h5o2	=	ch2oh+c2h5o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
450	ch3oh+ch3co3	=	ch2oh+ch3co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
451	ch3oh+c2h3co3	=	ch2oh+c2h3co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
452	ch3oh+c2h5co3	=	ch2oh+c2h5co3h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
453	ch3oh+nc3h7o2	=	ch2oh+nc3h7o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
454	ch3oh+ic3h7o2	=	ch2oh+ic3h7o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
455	ch3oh+pc4h9o2	=	ch2oh+pc4h9o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
456	ch3oh+sc4h9o2	=	ch2oh+sc4h9o2h	6.300e+12	0.00	1.936e+04	1.000e+09	0.00	1.000e+04
457	c2h5+ho2	=	c2h5o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.
458	nc3h7+ho2	=	nc3h7o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.
459	ic3h7+ho2	=	ic3h7o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
460	pc4h9+ho2	=	pc4h9o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.
461	sc4h9+ho2	=	sc4h9o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.
462	c3h5+ho2	=	c3h5o+oh	3.200e+13	0.00	0.	2.000e+10	0.00	0.
463	c4h7+ho2	=	c4h7o+oh	2.000e+13	0.00	0.	1.000e+14	0.00	2.560e+04
464	ch3o2+ch3	=	ch3o+ch3o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
465	ch3o2+c2h5	=	ch3o+c2h5o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
466	ch3o2+nc3h7	=	ch3o+nc3h7o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
467	ch3o2+ic3h7	=	ch3o+ic3h7o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
468	ch3o2+pc4h9	=	ch3o+pc4h9o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
469	ch3o2+sc4h9	=	ch3o+sc4h9o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
470	c3h5+ch3o2	=	c3h5o+ch3o	1.000e+13	0.00	0.	2.000e+10	0.00	0.
471	c4h7+ch3o2	=	c4h7o+ch3o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
472	ch3o2+ho2	=	ch3o2h+o2	9.200e+10	0.00	-2.600e+03	6.000e+12	0.00	3.900e+04
473	ch3o2+ho2	=	ch3o+oh+o2	1.000e+12	0.00	0.	0.	0.00	0.
474	c2h5o2+ho2	=	c2h5o2h+o2	9.200e+10	0.00	-2.600e+03	6.000e+12	0.00	3.900e+04
475	nc3h7o2+ho2	=	nc3h7o2h+o2	2.000e+12	0.00	0.	6.000e+12	0.00	3.900e+04
476	ic3h7o2+ho2	=	ic3h7o2h+o2	2.000e+12	0.00	0.	6.000e+12	0.00	3.900e+04
477	pc4h9o2+ho2	=	pc4h9o2h+o2	2.000e+12	0.00	0.	6.000e+12	0.00	3.900e+04
478	sc4h9o2+ho2	=	sc4h9o2h+o2	2.000e+12	0.00	0.	6.000e+12	0.00	3.900e+04
479	c3h5o2+ho2	=	c3h5ooh+o2	1.000e+11	0.00	0.	3.020e+12	0.00	3.900e+04
480	ch3co3+ho2	=	ch3co3h+o2	1.000e+12	0.00	0.	3.000e+12	0.00	3.900e+04
481	ch3co3+ho2	=	ch3co2+oh+o2	1.000e+12	0.00	0.	0.	0.00	0.
482	c2h5co3+ho2	=	c2h5co3h+o2	1.000e+12	0.00	0.	3.000e+12	0.00	3.900e+04
483	ch3o2+ch3o2	=	ch2o+ch3oh+o2	1.800e+12	0.00	0.	0.	0.00	0.
484	ch3o2+ch3o2	=	o2+ch3o+ch3o	1.850e+12	0.00	2.200e+03	0.	0.00	0.
485	ch3co3+ch3o2	=	ch3co2+ch3o+o2	9.000e+11	0.00	0.	0.	0.00	0.
486	ch3co3+ho2	=	ch3co2+oh+o2	1.000e+12	0.00	0.	0.	0.00	0.
487	ch3co3+ch3co3	=	o2+ch3co2+ch3co2	9.000e+11	0.00	0.	0.	0.00	0.
488	c4h10	=	c2h5+c2h5	1.100e+16	0.00	8.130e+04	3.980e+12	0.00	0.
489	c4h10	=	nc3h7+ch3	1.738e+17	0.00	8.570e+04	2.000e+13	0.00	0.
490	c4h10+o2	=	pc4h9+ho2	2.500e+13	0.00	4.900e+04	2.500e+12	0.00	-2.200e+03
491	c4h10+o2	=	sc4h9+ho2	4.000e+13	0.00	4.760e+04	4.070e+12	0.00	-3.622e+03
492	c4h10+h	=	pc4h9+h2	5.628e+07	2.00	7.700e+03	9.120e+12	0.00	1.446e+04
493	c4h10+h	=	sc4h9+h2	1.755e+07	2.00	5.000e+03	1.540e+13	0.00	1.587e+04
494	c4h10+oh	=	pc4h9+h2o	4.130e+07	1.73	7.530e+02	7.170e+07	1.73	2.227e+04
495	c4h10+oh	=	sc4h9+h2o	7.230e+07	1.64	-2.470e+02	1.280e+08	1.64	2.127e+04
496	c4h10+o	=	pc4h9+oh	1.130e+14	0.00	7.850e+03	1.480e+13	0.00	1.224e+04
497	c4h10+o	=	sc4h9+oh	5.620e+13	0.00	5.200e+03	7.350e+12	0.00	9.590e+03
498	c4h10+ch3	=	pc4h9+ch4	2.189e+11	0.00	1.140e+04	5.555e+12	0.00	1.856e+04
499	c4h10+ch3	=	sc4h9+ch4	2.189e+11	0.00	9.600e+03	3.432e+12	0.00	1.646e+04
500	c4h10+c2h3	=	pc4h9+c2h4	1.000e+12	0.00	1.800e+04	2.570e+12	0.00	2.538e+04
501	c4h10+c2h3	=	sc4h9+c2h4	8.000e+11	0.00	1.680e+04	2.050e+12	0.00	2.418e+04
502	c4h10+c2h5	=	pc4h9+c2h6	1.580e+11	0.00	1.230e+04	3.560e+10	0.00	1.292e+04
503	c4h10+c2h5	=	sc4h9+c2h6	1.000e+11	0.00	1.040e+04	7.120e+10	0.00	9.917e+03
504	c4h10+c3h5	=	pc4h9+c3h6	7.940e+11	0.00	2.050e+04	1.000e+12	0.00	2.000e+04
505	c4h10+c3h5	=	sc4h9+c3h6	3.160e+11	0.00	1.640e+04	1.000e+12	0.00	2.000e+04
506	c4h10+ho2	=	pc4h9+h2o2	1.700e+13	0.00	2.046e+04	4.580e+12	0.00	9.809e+03
507	c4h10+ho2	=	sc4h9+h2o2	4.000e+12	0.00	1.815e+04	1.630e+12	0.00	7.409e+03
508	c4h10+ch3o	=	pc4h9+ch3oh	3.000e+11	0.00	7.000e+03	1.220e+10	0.00	5.000e+04
509	c4h10+ch3o	=	sc4h9+ch3oh	6.000e+11	0.00	7.000e+03	2.441e+10	0.00	5.000e+04
510	pc4h9	=	c2h5+c2h4	2.500e+13	0.00	2.880e+04	3.000e+11	0.00	8.000e+03

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
511	pc4h9	=	1c4h8+h	1.260e+13	0.00	3.860e+04	7.940e+12	0.00	2.900e+03
512	pc4h9+o2	=	1c4h8+ho2	3.800e+10	0.00	-2.000e+03	2.850e+10	0.00	1.385e+04
513	sc4h9	=	2c4h8+h	5.010e+12	0.00	3.790e+04	1.000e+13	0.00	1.500e+03
514	sc4h9	=	1c4h8+h	2.000e+13	0.00	4.040e+04	1.000e+13	0.00	1.500e+03
515	sc4h9	=	c3h6+ch3	2.000e+14	0.00	3.320e+04	3.160e+11	0.00	7.400e+03
516	sc4h9+o2	=	1c4h8+ho2	7.590e+09	0.00	-2.000e+03	5.640e+09	0.00	1.385e+04
517	sc4h9+o2	=	2c4h8+ho2	1.810e+10	0.00	-2.000e+03	1.340e+10	0.00	1.385e+04
518	c3h6+ho2	=	c3h5+h2o2	3.000e+12	0.00	1.700e+04	1.000e+12	0.00	7.500e+03
519	c2h4+ch3	=	c2h3+ch4	1.000e+13	0.00	1.100e+04	3.030e+13	0.00	1.258e+04
520	c2h3co	=	c2h3+co	8.600e+15	0.00	2.300e+04	1.585e+11	0.00	6.000e+03
521	ch3co3h	=	ch3+co2+oh	2.000e+14	0.00	4.015e+04	0.	0.00	0.
522	pc4h9o2	=	ch2ch2ch2ch2o2h	2.200e+08	0.00	1.900e+04	7.300e+07	0.00	1.100e+04
523	pc4h9o2	=	ch3chch2ch2o2h	5.200e+08	0.00	1.730e+04	8.500e+07	0.00	1.290e+04
524	pc4h9o2	=	ch3ch2chch2o2h	6.500e+08	0.00	2.040e+04	3.200e+08	0.00	1.590e+04
525	sc4h9o2	=	ch2ch2cho2hch3	5.200e+08	0.00	2.090e+04	1.700e+08	0.00	1.290e+04
526	sc4h9o2	=	ch3chcho2hch3	6.500e+08	0.00	2.040e+04	3.200e+08	0.00	1.590e+04
527	ch2ch2ch2ch2o2h	=	(c4h8o-c)+oh	1.000e+12	0.00	2.000e+04	1.000e+11	0.00	5.000e+04
528	ch3chch2ch2o2h	=	(c4h8o-2mo)+oh	1.000e+12	0.00	2.000e+04	1.000e+11	0.00	5.000e+04
529	ch3cho2ch2ch2o2h	=	ch3chch2ch2o2h+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.
530	reaction index skipped.								
531	reaction index skipped.								
532	ch3ch2chch2o2h	=	ch2ochch2ch3+oh	1.000e+12	0.00	2.000e+04	1.000e+11	0.00	5.000e+04
533	ch2ch2cho2hch3	=	(c4h8o-2mo)+oh	1.000e+12	0.00	2.000e+04	6.200e+10	0.00	1.890e+04
534	o2ch2ch2cho2hch3	=	ch2ch2cho2hch3+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0
535	o2ch2ch2cho2hch3	=	ch3cho+ch2o+ch2o2h	0.	0.00	4.300e+04	0.	0.00	0.
536	ch2ochch2ch3+oh	=	ch2ochchch3+h2o	4.670e+07	1.61	-3.500e+01	8.300e+07	1.61	2.150e+04
537	ch3chcho2hch3	=	ch3chochch3+oh	1.000e+12	0.00	2.000e+04	1.000e+11	0.00	5.000e+04
538	ch3cho2cho2hch3	=	ch3chcho2hch3+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.
539	reaction index skipped.								
540	(c4h8o-2mo)+oh	=	(c4h7o-2mo)+h2o	5.270e+09	0.97	1.586e+03	5.000e+08	1.25	2.240e+04
541	(c4h8o-2mo)+h	=	(c4h7o-2mo)+h2	2.810e+07	2.00	7.700e+03	9.000e+12	0.00	1.450e+04
542	(c4h8o-2mo)+ho2	=	(c4h7o-2mo)+h2o2	6.500e+12	0.00	2.046e+04	1.200e+12	0.00	9.800e+03
543	(c4h7o-2mo)	=	c3h5+ch2o	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
544	(c4h7o-2mo)	=	ch2cho+c2h4	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
545	ch2ochch2ch3+oh	=	ch2ochch2ch2+h2o	5.270e+09	0.97	1.586e+03	5.000e+08	1.25	2.240e+04
546	ch2ochch2ch3+h	=	ch2ochch2ch2+h2	2.810e+07	2.00	7.700e+03	9.000e+12	0.00	1.450e+04
547	ch2ochch2ch3+ho2	=	ch2ochch2ch2+h2o2	6.500e+12	0.00	2.046e+04	1.200e+12	0.00	9.800e+03
548	ch2ochch2ch2	=	ch2cho+c2h4	9.600e+13	0.00	3.100e+04	1.000e+11	0.00	4.000e+03
549	ch2ochch2ch3+oh	=	ch2ochchch3+h2o	4.670e+07	1.61	-3.500e+01	8.300e+07	1.61	2.150e+04
550	ch2ochch2ch3+h	=	ch2ochchch3+h2	8.775e+06	2.00	5.000e+03	7.700e+12	0.00	1.600e+04
551	ch2ochch2ch3+ho2	=	ch2ochchch3+h2o2	2.000e+12	0.00	1.700e+04	4.000e+11	0.00	7.500e+03
552	ch2ochchch3	=	chchch3+ch2o	1.000e+15	0.00	2.160e+04	1.000e+07	1.00	1.360e+04
553	chchch3+o2	=	ch3cho+hco	4.000e+12	0.00	-2.500e+02	3.900e+12	0.00	8.600e+04
554	chchch3	=	c2h2+ch3	9.600e+13	0.00	3.100e+04	1.000e+11	0.00	4.000e+03
555	ch3chochch3+oh	=	ch3chochch2+h2o	5.270e+09	0.97	1.586e+03	5.000e+08	1.25	2.240e+04
556	ch3chochch3+h	=	ch3chochch2+h2	2.810e+07	2.00	7.700e+03	9.000e+12	0.00	1.450e+04
557	ch3chochch3+ho2	=	ch3chochch2+h2o2	6.500e+12	0.00	2.046e+04	1.200e+12	0.00	9.800e+03
558	ch3chochch2	=	ch3cho+c2h3	7.940e+14	0.00	1.530e+04	1.000e+10	0.00	2.000e+04
559	1c4h8oh	=	1c4h8+oh	1.500e+13	0.00	2.583e+04	4.750e+12	0.00	-7.820e+02
560	2c4h8oh	=	2c4h8+oh	1.500e+13	0.00	2.583e+04	4.750e+12	0.00	-7.820e+02
561	1o2c4h8oh	=	1c4h8oh+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
562	2o2c4h8oh	=	2c4h8oh+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.
563	1o2c4h8oh	=	c2h5cho+ch2o+oh	1.000e+16	0.00	2.500e+04	0.	0.00	0.
564	2o2c4h8oh	=	oh+ch3cho+ch3cho	1.000e+16	0.00	2.500e+04	0.	0.00	0.
565	c4h7+c2h5o2	=	c4h7o+c2h5o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
566	c4h7+pc4h9o2	=	c4h7o+pc4h9o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
567	c4h7+sc4h9o2	=	c4h7o+sc4h9o	3.800e+12	0.00	-1.200e+03	2.000e+10	0.00	0.
568	c4h7o	=	ch3cho+c2h3	7.940e+14	0.00	1.900e+04	1.000e+10	0.00	2.000e+04
569	c4h7o	=	c2h3cho+ch3	7.940e+14	0.00	1.900e+04	1.000e+10	0.00	2.000e+04
570	ch2cho	=	ch2co+h	1.600e+13	0.00	3.500e+04	1.000e+14	0.00	1.600e+04
571	hcco+o2	=	oh+co+co	1.460e+12	0.00	2.500e+03	0.	0.00	0.
572	c2h5co	=	c2h5+co	1.000e+14	0.00	1.050e+04	3.000e+09	1.00	7.471e+03
573	ch2cho+o2	=	ch2co+ho2	1.810e+11	0.00	1.840e+03	7.151e+10	0.00	3.385e+03
574	c4h10+c2h5o	=	pc4h9+c2h5oh	3.000e+11	0.00	7.000e+03	1.000e+10	0.00	5.000e+04
575	c4h10+c2h5o	=	sc4h9+c2h5oh	7.200e+10	0.00	4.500e+03	1.000e+10	0.00	5.000e+04
576	1c4h8+ho2	=	c4h7+h2o2	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
577	1c4h8+ch3o2	=	c4h7+ch3o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
578	1c4h8+c2h5o2	=	c4h7+c2h5o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
579	1c4h8+nc3h7o2	=	c4h7+nc3h7o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
580	1c4h8+ic3h7o2	=	c4h7+ic3h7o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
581	1c4h8+pc4h9o2	=	c4h7+pc4h9o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
582	1c4h8+sc4h9o2	=	c4h7+sc4h9o2h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
583	1c4h8+c2h3co3	=	c4h7+c2h3co3h	1.400e+12	0.00	1.490e+04	3.160e+11	0.00	1.300e+04
584	2c4h8+ho2	=	c4h7+h2o2	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
585	2c4h8+ch3o2	=	c4h7+ch3o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
586	2c4h8+c2h5o2	=	c4h7+c2h5o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
587	2c4h8+nc3h7o2	=	c4h7+nc3h7o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
588	2c4h8+ic3h7o2	=	c4h7+ic3h7o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
589	2c4h8+pc4h9o2	=	c4h7+pc4h9o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
590	2c4h8+sc4h9o2	=	c4h7+sc4h9o2h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
591	2c4h8+c2h3co3	=	c4h7+c2h3co3h	3.200e+12	0.00	1.490e+04	1.585e+11	0.00	1.470e+04
592	1c4h8+ho2	=	ch2ochch2ch3+oh	1.290e+12	0.00	1.490e+04	0.	0.00	0.
593	2c4h8+ho2	=	ch3chochch3+oh	1.290e+12	0.00	1.490e+04	0.	0.00	0.
594	1c4h8+o2	=	c4h7+ho2	2.700e+13	0.00	3.700e+04	3.000e+11	0.00	0.
595	2c4h8+o2	=	c4h7+ho2	8.000e+13	0.00	4.000e+04	3.000e+11	0.00	0.
596	c2h6+c2h5o2	=	c2h5+c2h5o2h	1.700e+13	0.00	2.046e+03	5.000e+11	0.00	6.500e+03
597	c2h5o2+c2h5o2	=	o2+c2h5o+c2h5o	1.857e+12	0.00	2.200e+03	0.	0.00	0.
598	c3h6+o2	=	c3h5+ho2	1.000e+14	0.00	3.900e+04	1.000e+12	0.00	0.
599	ch3+oh	=	ch2+h2o	1.500e+13	0.00	5.000e+03	1.312e+13	0.00	1.545e+04
600	reaction index skipped.								
601	ch3cho2ch2ch2o2h	=	ch3cho2hch2cho2h	8.200e+10	0.00	1.850e+04	4.100e+10	0.00	1.900e+04
602	ch3cho2cho2hch3	=	ch3cho2hco2hch3	7.600e+10	0.00	2.250e+04	7.600e+10	0.00	2.200e+04
603	ch3cho2hch2cho2h	=	ch3cho+ch2cho+oh+oh	8.400e+14	0.00	2.600e+04	0.	0.00	0.
604	ch3cho2hco2hch3	=	ch3cho+ch3co+oh+oh	8.400e+14	0.00	2.600e+04	0.	0.00	0.
605	c2h5o	=	ch3cho+h	2.510e+14	0.00	2.340e+04	1.000e+12	0.00	0.
606	ic3h7o	=	ch3coch3+h	2.000e+14	0.00	2.150e+04	1.000e+12	0.00	0.
607	pc4h9o	=c3h7cho+h		2.510e+14	0.00	2.340e+04	1.000e+12	0.00	0.
608	sc4h9o	=ch3ch2coch3+h		2.000e+14	0.00	2.150e+04	1.000e+12	0.00	0.
609	c3h6oh	=	c3h6+oh	1.500e+15	0.00	2.780e+04	2.760e+12	0.00	-1.042e+03
610	hoc3h6o2	=	c3h6oh+o2	3.270e+17	-1.00	3.000e+04	1.000e+12	0.00	-1.100e+03
611	hoc3h6o2	=	ch3cho+ch2o+oh	1.000e+16	0.00	2.500e+04	0.	0.00	0.
612	nc5h12	=	ch3+pc4h9	4.725e+19	-1.00	8.714e+04	1.995e+13	0.00	0.

	Reaction			Forward rate			Reverse rate		
				A	n	Ea	A	n	Ea
613	nc5h12	=	nc3h7+c2h5	6.310e+16	0.00	8.190e+04	7.940e+12	0.00	0.
614	nc5h12+o2	=	1c5h11+ho2	2.500e+13	0.00	4.900e+04	2.500e+12	0.00	0.
615	nc5h12+o2	=	2c5h11+ho2	4.000e+13	0.00	4.760e+04	4.000e+12	0.00	0.
616	nc5h12+o2	=	3c5h11+ho2	2.000e+13	0.00	4.760e+04	4.000e+12	0.00	0.
617	nc5h12+h	=	1c5h11+h2	5.600e+07	2.00	7.700e+03	3.200e+12	0.00	1.570e+04
618	nc5h12+h	=	2c5h11+h2	1.800e+07	2.00	5.000e+03	5.000e+12	0.00	1.720e+04
619	nc5h12+h	=	3c5h11+h2	8.800e+06	2.00	5.000e+03	5.000e+12	0.00	1.720e+04
620	nc5h12+oh	=	1c5h11+h2o	8.600e+09	1.05	1.810e+03	1.700e+10	1.05	2.390e+04
621	nc5h12+oh	=	2c5h11+h2o	2.600e+09	1.25	7.030e+02	4.600e+09	1.25	2.220e+04
622	nc5h12+oh	=	3c5h11+h2o	1.300e+09	1.25	7.030e+02	4.600e+09	1.25	2.220e+04
623	nc5h12+o	=	1c5h11+oh	1.130e+14	0.00	7.850e+03	1.500e+13	0.00	1.220e+04
624	nc5h12+o	=	2c5h11+oh	5.620e+13	0.00	5.200e+03	7.000e+12	0.00	9.600e+03
625	nc5h12+o	=	3c5h11+oh	2.800e+13	0.00	5.200e+03	7.000e+12	0.00	9.600e+03
626	nc5h12+ch3	=	1c5h11+ch4	1.300e+12	0.00	1.160e+04	2.510e+11	0.00	1.760e+04
627	nc5h12+ch3	=	2c5h11+ch4	8.000e+11	0.00	9.500e+03	5.000e+11	0.00	1.960e+04
628	nc5h12+ch3	=	3c5h11+ch4	4.000e+11	0.00	9.500e+03	5.000e+11	0.00	1.960e+04
629	nc5h12+ho2	=	1c5h11+h2o2	1.700e+13	0.00	2.046e+04	4.600e+12	0.00	9.810e+03
630	nc5h12+ho2	=	2c5h11+h2o2	6.700e+12	0.00	1.700e+04	2.700e+12	0.00	7.410e+03
631	nc5h12+ho2	=	3c5h11+h2o2	3.300e+12	0.00	1.700e+04	2.700e+12	0.00	7.410e+03
632	nc5h12+c2h5	=	1c5h11+c2h6	1.000e+11	0.00	1.340e+04	3.200e+11	0.00	1.230e+04
633	nc5h12+c2h5	=	2c5h11+c2h6	1.000e+11	0.00	1.040e+04	1.000e+11	0.00	1.290e+04
634	nc5h12+c2h5	=	3c5h11+c2h6	5.000e+10	0.00	1.040e+04	1.000e+11	0.00	1.290e+04
635	nc5h12+c2h3	=	1c5h11+c2h4	1.000e+12	0.00	1.800e+04	2.600e+12	0.00	2.540e+04
636	nc5h12+c2h3	=	2c5h11+c2h4	8.000e+11	0.00	1.680e+04	2.000e+12	0.00	2.420e+04
637	nc5h12+c2h3	=	3c5h11+c2h4	4.000e+11	0.00	1.680e+04	1.000e+12	0.00	2.420e+04
638	nc5h12+pc4h9	=	1c5h11+c4h10	3.200e+11	0.00	1.230e+04	3.200e+11	0.00	1.230e+04
639	nc5h12+pc4h9	=	2c5h11+c4h10	1.000e+11	0.00	1.040e+04	1.000e+11	0.00	1.290e+04
640	nc5h12+pc4h9	=	3c5h11+c4h10	5.000e+11	0.00	1.040e+04	1.000e+11	0.00	1.290e+04
641	nc5h12+sc4h9	=	1c5h11+c4h10	1.000e+11	0.00	1.290e+04	1.000e+11	0.00	1.040e+04
642	nc5h12+sc4h9	=	2c5h11+c4h10	1.000e+11	0.00	1.230e+04	1.000e+11	0.00	1.230e+04
643	nc5h12+sc4h9	=	3c5h11+c4h10	5.000e+10	0.00	1.230e+04	1.000e+11	0.00	1.230e+04
644	nc5h12+ch3o	=	1c5h11+ch3oh	3.000e+11	0.00	7.000e+03	1.200e+10	0.00	9.200e+03
645	nc5h12+ch3o	=	2c5h11+ch3oh	2.200e+11	0.00	5.000e+03	9.000e+09	0.00	7.200e+03
646	nc5h12+ch3o	=	3c5h11+ch3oh	1.100e+11	0.00	5.000e+03	9.000e+09	0.00	7.200e+03
647	1c5h11	=	c2h4+nc3h7	3.200e+13	0.00	2.840e+04	6.300e+10	0.00	7.400e+03
648	1c5h11	=	h+1c5h10	1.300e+13	0.00	3.860e+04	7.900e+12	0.00	2.900e+03
649	2c5h11	=	c3h6+c2h5	5.000e+12	0.00	2.910e+04	4.000e+10	0.00	7.500e+03
650	2c5h11	=	1c5h10+h	2.000e+13	0.00	4.040e+04	7.900e+12	0.00	2.900e+03
651	2c5h11	=	2c5h10+h	5.000e+12	0.00	3.790e+04	2.500e+12	0.00	1.200e+03
652	3c5h11	=	1c4h8+ch3	1.600e+14	0.00	3.300e+04	2.000e+11	0.00	7.200e+03
653	3c5h11	=	2c5h10+h	1.000e+13	0.00	3.790e+04	2.500e+12	0.00	1.200e+03
654	1c5h11	=	2c5h11	2.000e+11	0.00	1.810e+04	3.000e+11	0.00	2.110e+04
655	1c5h11+o2	=	1c5h10+ho2	1.000e+12	0.00	2.000e+03	2.000e+11	0.00	1.590e+04
656	2c5h11+o2	=	1c5h10+ho2	1.000e+12	0.00	4.500e+03	2.000e+11	0.00	1.840e+04
657	2c5h11+o2	=	2c5h10+ho2	2.000e+12	0.00	4.250e+03	4.000e+11	0.00	1.810e+04
658	3c5h11+o2	=	2c5h10+ho2	2.000e+12	0.00	4.250e+03	4.000e+11	0.00	1.810e+04
659	pc4h9o2+pc4h9o2	=o2+pc4h9o+pc4h9o		5.000e+11	0.00	0.	0.	0.00	0.
660	pc4h9o2+sc4h9o2	=o2+pc4h9o+sc4h9o		5.000e+11	0.00	0.	0.	0.00	0.
661	pc4h9o2+c2h5o2	=o2+pc4h9o+c2h5o		5.000e+11	0.00	0.	0.	0.00	0.
662	pc4h9o2+ch3o2	=o2+pc4h9o+ch3o		5.000e+11	0.00	0.	0.	0.00	0.
663	pc4h9o2+ch3co3	=o2+pc4h9o+ch3co2		5.000e+11	0.00	0.	0.	0.00	0.

		Reaction	Forward rate A	n	Ea	Reverse rate A	n	Ea
664	pc4h9o2+c2h3co3	=o2+pc4h9o+c2h3co2	5.000e+11	0.00	0.	0.	0.00	0.
665	sc4h9o2+sc4h9o2	=o2+sc4h9o+sc4h9o	5.000e+11	0.00	0.	0.	0.00	0.
666	sc4h9o2+c2h5o2	=o2+sc4h9o+c2h5o	5.000e+11	0.00	0.	0.	0.00	0.
667	sc4h9o2+ch3o2	=o2+sc4h9o+ch3o	5.000e+11	0.00	0.	0.	0.00	0.
668	sc4h9o2+ch3co3	=o2+sc4h9o+ch3co2	5.000e+11	0.00	0.	0.	0.00	0.
669	sc4h9o2+c2h3co3	=o2+sc4h9o+c2h3co2	5.000e+11	0.00	0.	0.	0.00	0.
670	1c4h8+c4h6	=c4h7+c4h7	2.350e+12	0.00	4.672e+04	1.600e+12	0.00	0.
671	2c4h8+c4h6	=c4h7+c4h7	2.350e+12	0.00	4.672e+04	1.600e+12	0.00	0.
672	c4h7+ch3	=c4h6+ch4	8.000e+12	0.00	0.	7.050e+13	0.00	5.728e+04
673	h2o2+ch3o2	=ch3o2h+ho2	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
674	h2o2+c2h5o2	=c2h5o2h+ho2	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
675	h2o2+pc4h9o2	=pc4h9o2h+ho2	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
676	h2o2+sc4h9o2	=sc4h9o2h+ho2	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
677	c2h5o2+ho2	=c2h5o+oh+o2	1.000e+11	0.00	0.	0.	0.00	0.
678	nc3h7o2+ho2	=nc3h7o+oh+o2	1.000e+11	0.00	0.	0.	0.00	0.
679	ic3h7o2+ho2	=ic3h7o+oh+o2	1.000e+11	0.00	0.	0.	0.00	0.
680	pc4h9o2+ho2	=pc4h9o+oh+o2	1.000e+11	0.00	0.	0.	0.00	0.
681	sc4h9o2+ho2	=sc4h9o+oh+o2	1.000e+11	0.00	0.	0.	0.00	0.
682	h2o2+nc3h7o2	=ho2+nc3h7o2h	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
683	h2o2+ic3h7o2	=ho2+ic3h7o2h	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
684	h2o2+ch3co3	=ho2+ch3co3h	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
685	h2o2+c2h3co3	=ho2+c2h3co3h	2.400e+12	0.00	1.000e+04	2.400e+12	0.00	1.000e+04
686	pc4h9o2+nc3h7o2	=pc4h9o+nc3h7o+o2	5.000e+11	0.00	0.	0.	0.00	0.
687	pc4h9o2+ic3h7o2	=pc4h9o+ic3h7o+o2	5.000e+11	0.00	0.	0.	0.00	0.
688	sc4h9o2+nc3h7	=sc4h9o+nc3h7o+o2	5.000e+11	0.00	0.	0.	0.00	0.
689	sc4h9o2+ic3h7	=sc4h9o+ic3h7o+o2	5.000e+11	0.00	0.	0.	0.00	0.
690	ch3ch2cho2ch2o2h	=ch3ch2chch2o2h+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.
691	ch3ch2cho2ch2o2h	=ch3ch2cho2hcho2h	1.900e+11	0.00	3.000e+04	1.900e+11	0.00	2.200e+04
692	o2ch2ch2cho2hch3	=ho2ch2ch2co2hch3	6.200e+10	0.00	2.340e+04	6.200e+10	0.00	1.890e+04
693	ch3ch2cho2hcho2h	=c2h5cho+hco+oh+oh	8.400e+14	0.00	2.600e+04	0.	0.00	0.
694	ho2ch2ch2co2hch3	=ch3coch2+ch2o+oh+oh	8.400e+14	0.00	2.600e+04	0.	0.00	0.
695	c4h8o-c+oh	=c4h7o-c+h2o	1.870e+08	1.61	-3.500e+01	1.230e+08	1.61	2.163e+04
696	c4h7o-c	=c2h4+ch2cho	1.000e+13	0.00	2.000e+04	1.000e+10	0.00	5.000e+04
697	c4h7o-c	=c3h5+ch2o	1.000e+13	0.00	2.000e+04	1.000e+10	0.00	5.000e+04
698	c8h14	=c4h7+c4h7	6.310e+15	0.00	5.660e+04	4.000e+12	0.00	0.
699	c8h14oh	=c8h14+oh	1.500e+13	0.00	2.583e+04	4.750e+12	0.00	-7.820e+02
700	o2c8h14oh	=c8h14oh+o2	4.390e+18	-1.00	3.702e+04	1.000e+12	0.00	0.
701	o2c8h14oh	=ch3+c2h3cho+ch3cho+ch3cho	1.000e+16	0.00	2.500e+04	0.	0.00	0.

"Unimolecular" reactions in fall-off regions.

	reaction			arc	arp	arx
1	ch4	=	ch3+h	6.3000e-03	0.00	1.8000e+04
15	c2h5	=	c2h4+h	3.4700e-12	2.76	2.1200e+03
24	c2h6	=	ch3+ch3	7.6600e-07	0.00	3.0320e+03
60	c2h3	=	c2h2+h	3.7200e-09	1.12	0.